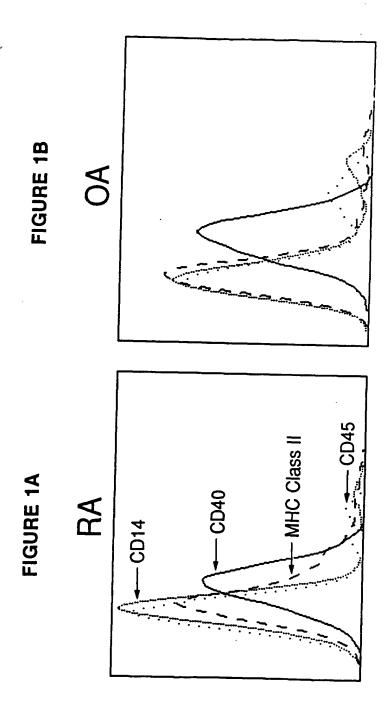
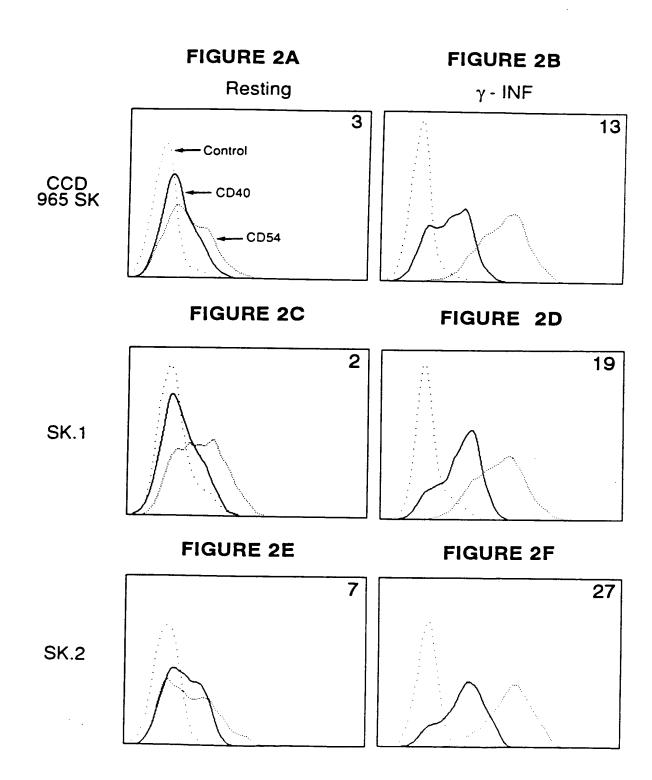
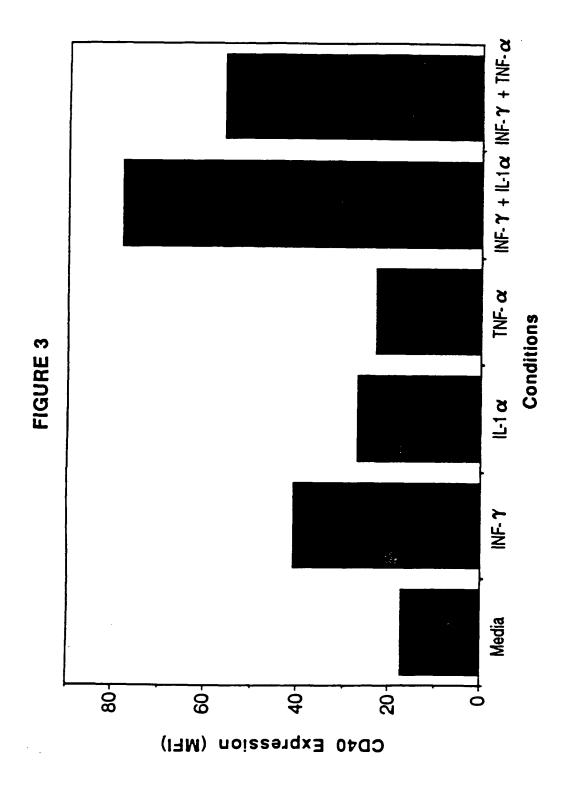
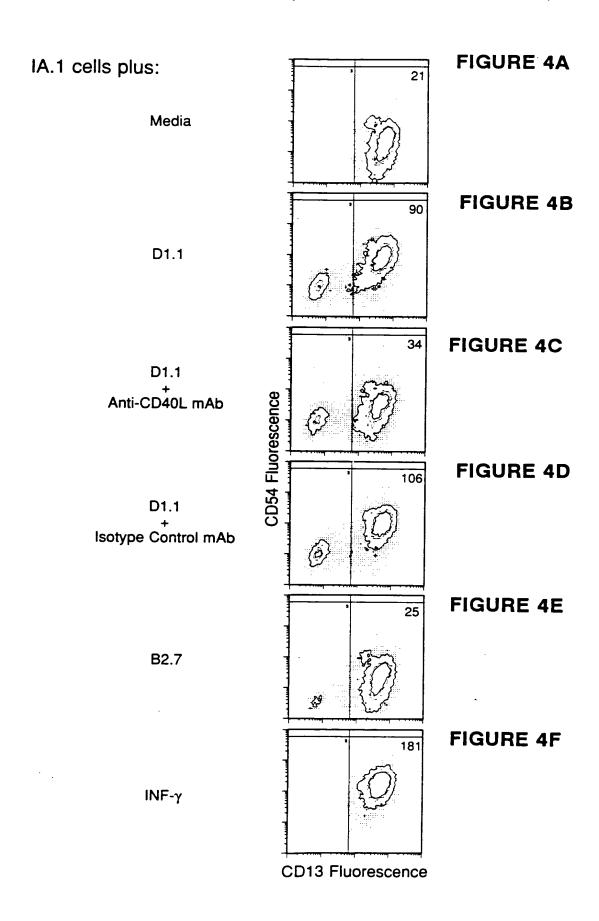
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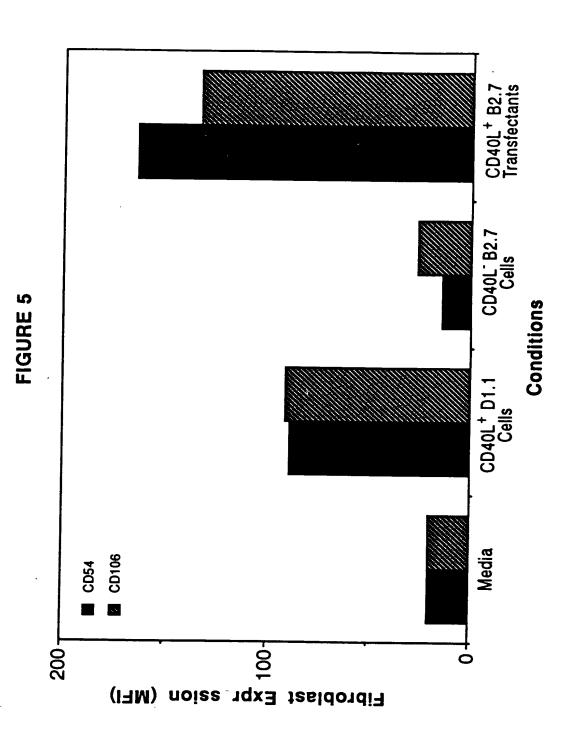




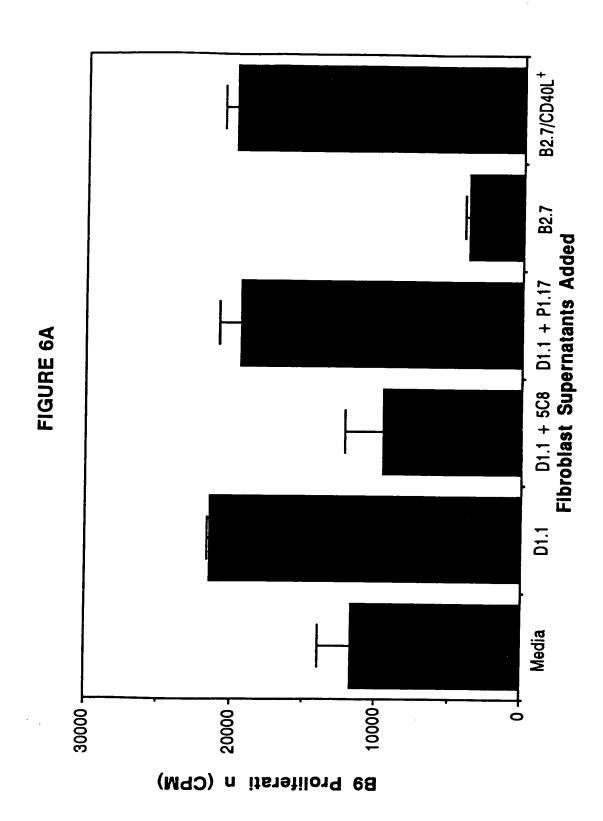




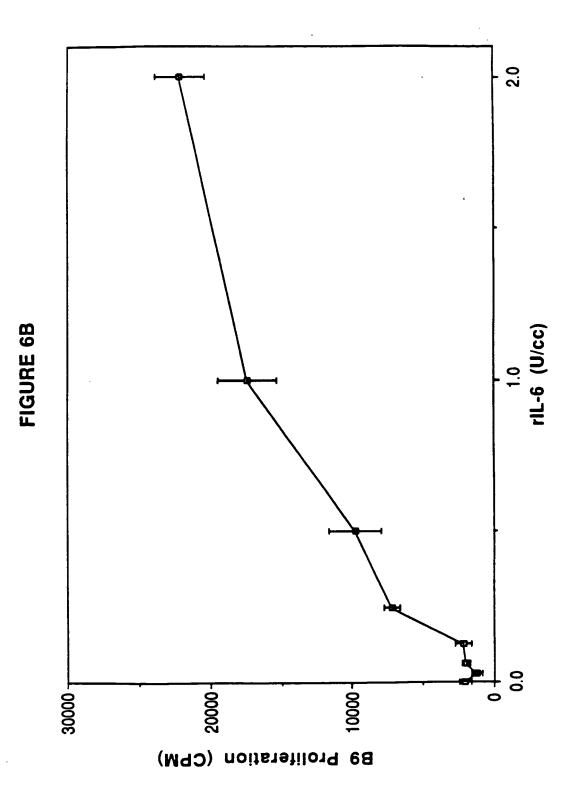




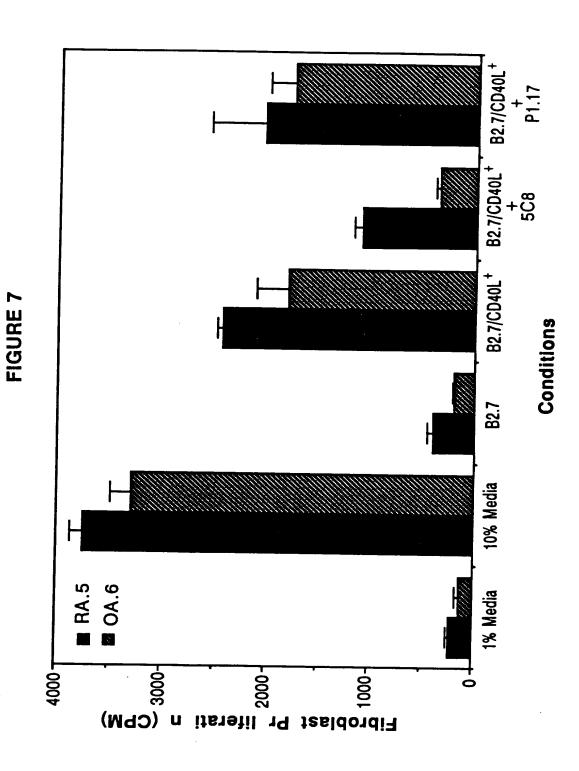












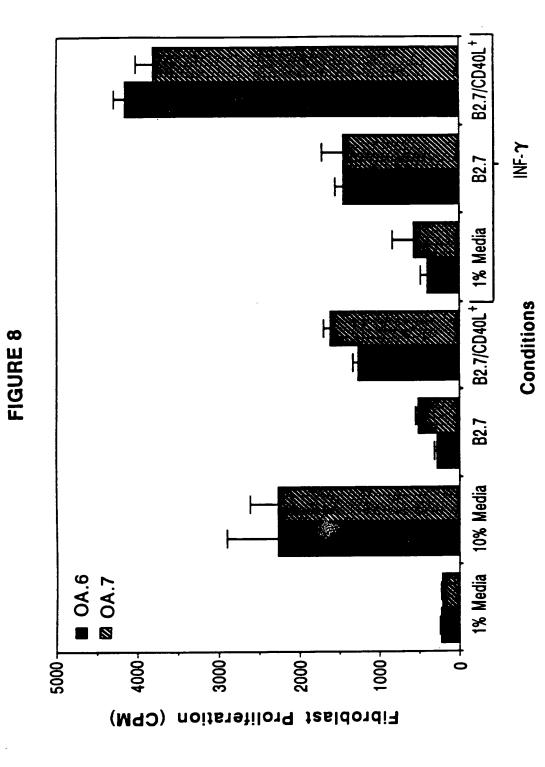
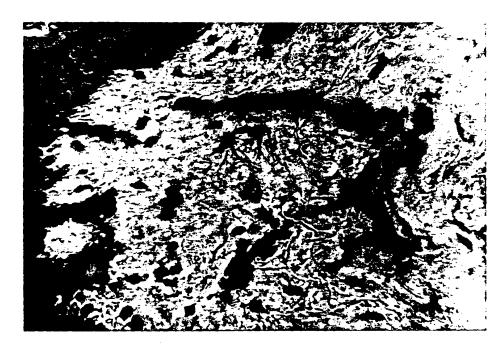
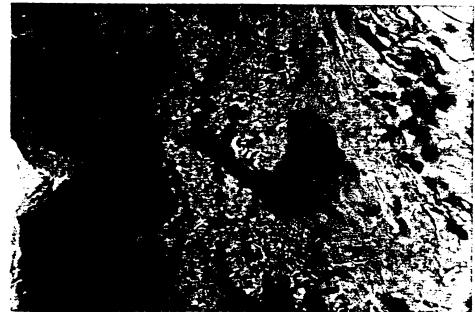




FIGURE 9B





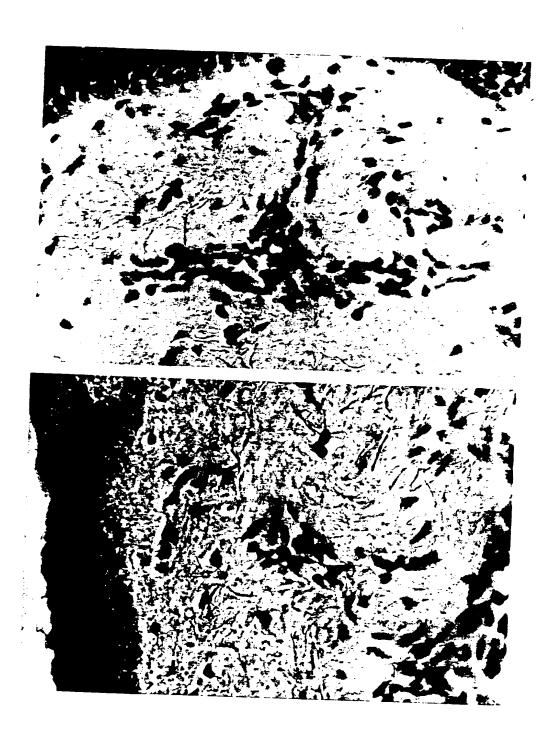
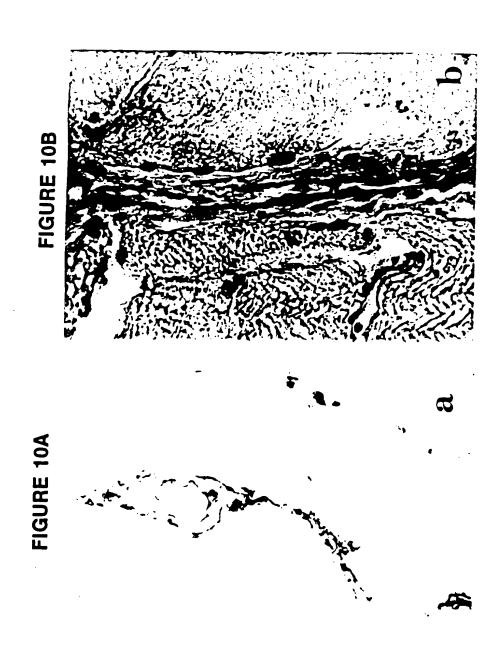


FIGURE 9C

FIGURE 9D



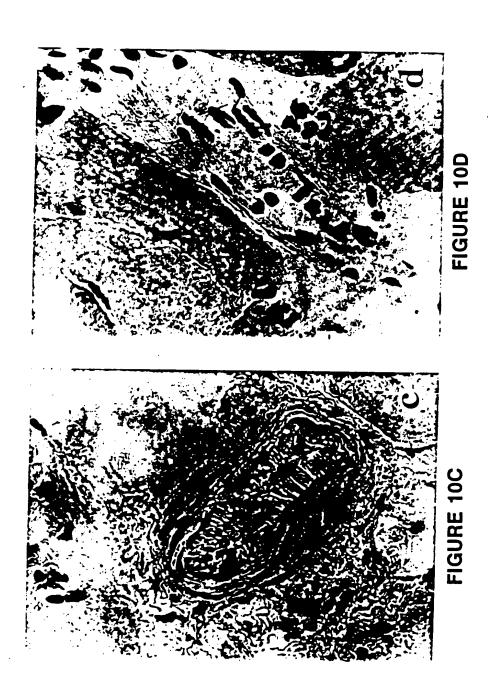


FIGURE 11B

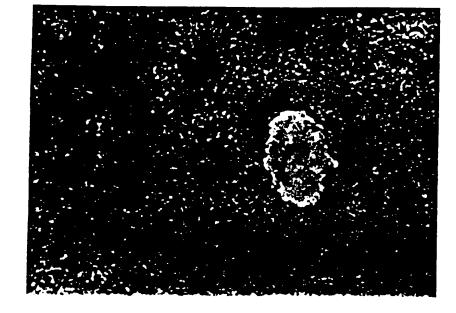
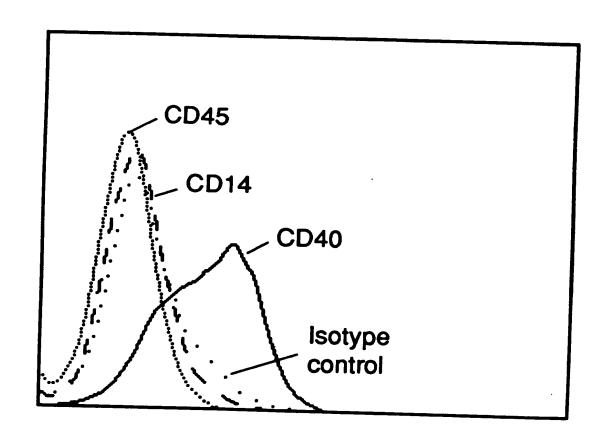


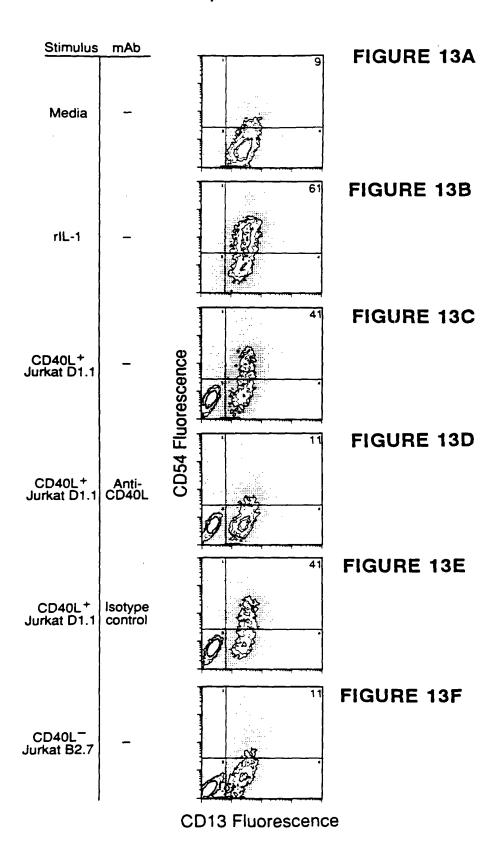
FIGURE 11A



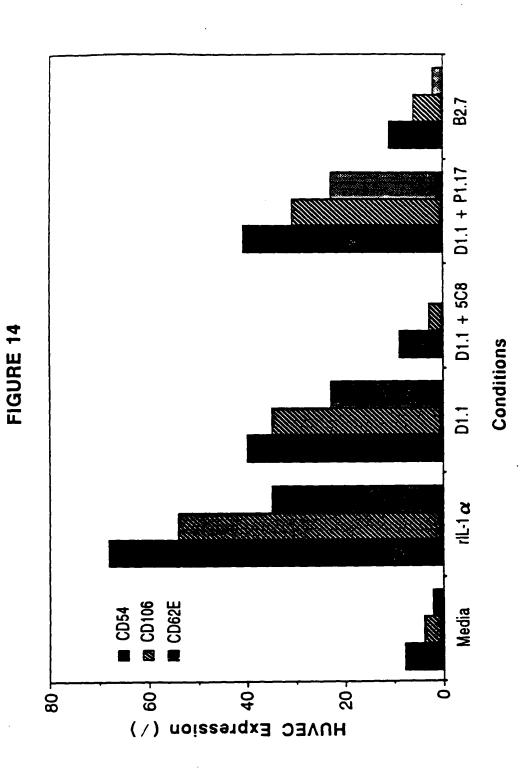
FIGURE 12

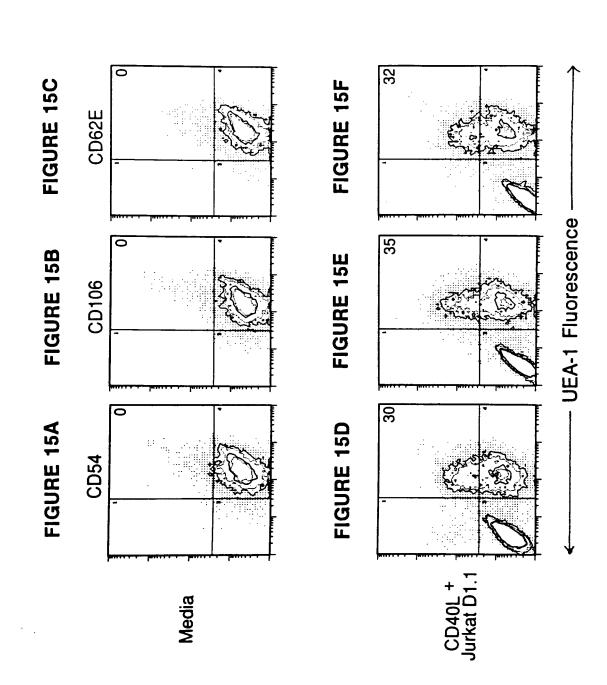


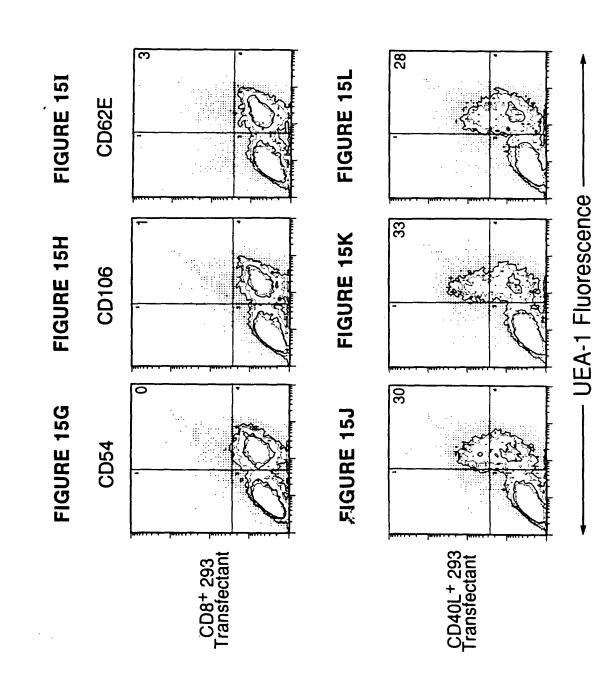
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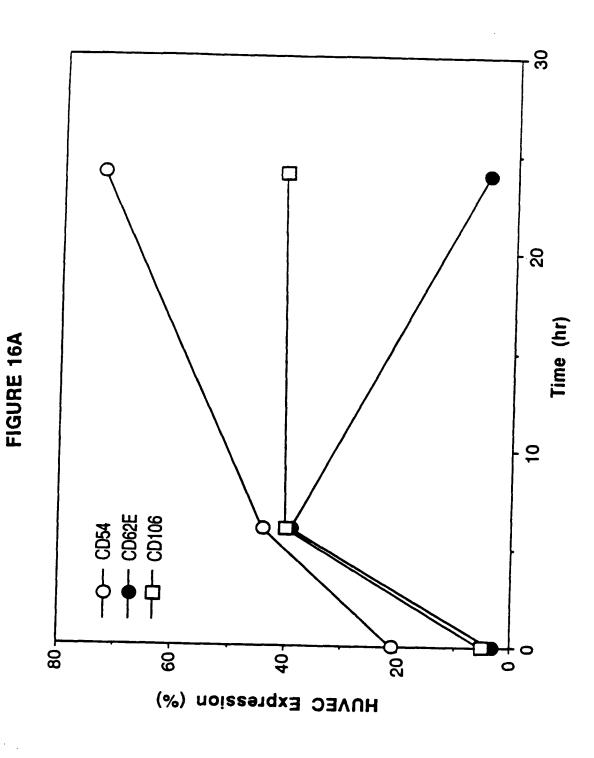












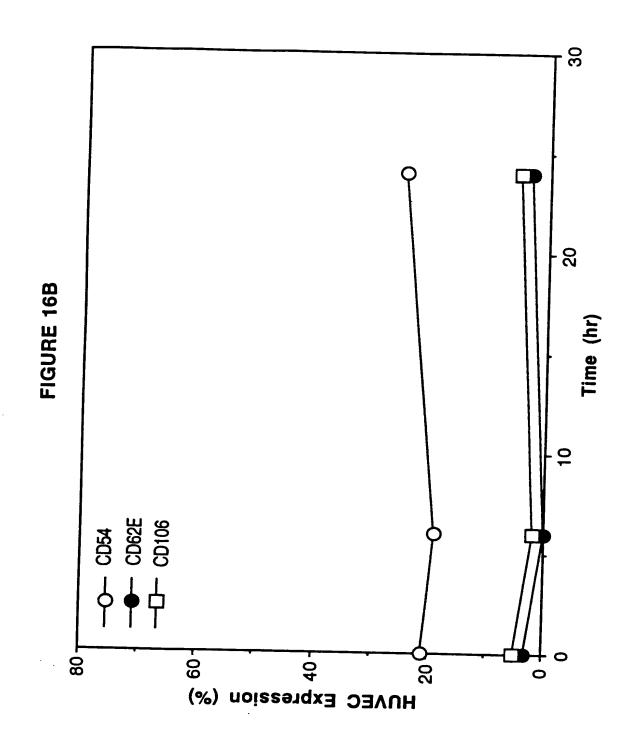


FIGURE 17A

| | | | | | | | | | | - | |
|--------------|-----|-----------|------------|------------|--------|-------|------------------|------------------|--------|----------------|--------|
| REM' RKS | ATC | MIC C | | | OF CD4 | | | RUCTURE | IN PDB | FORMAT | - |
| CKYST | 77 | .170 | 77. | 170 | 90.460 | 90. | 00 90.0 | 0 120.00 | R3 | | |
| ATOM | 1 | . N | GLY | 116 | | 7.954 | -16.144 | 22.488 | 1.00 | 64.71 | A |
| ATOM | 2 | HTl | GLY | 116 | | 7.087 | -15.852 | 21.964 | 1.00 | 15.00 | A |
| ATOM | 3 | HT2 | GLY | 116 | - 6 | 3.082 | -17.142 | 22.242 | 1.00 | 15.00 | A |
| ATOM | 4 | HT3 | GLY | 116 | - 8 | 3.630 | -15.576 | 21.928 | | | A |
| MOTA | 5 | CA | GLY | 116 | - 7 | 7.927 | -15.755 | 23.928 | 1.00 | 64.37 | A |
| ATOM | 6 | C | GLY | 116 | - 6 | . 990 | -16.621 | 24.780 | | 64.34 | A |
| ATOM | 7 | 0 | GLY | 116 | - 6 | . 968 | -17.814 | 24.563 | 1.00 | 64.44 | A |
| ATOM | 8 | N | ASP | 117 | - 6 | . 238 | -16.043 | 25.740 | 1.00 | 64.04 | A |
| ATOM | 9 | H | ASP | 117 | - 5 | 6.617 | -16.709 | 26.170 | 1.00 | 15.00 | A |
| ATOM | 10 | CA | ASP | 117 | - 6 | .284 | -14.616 | 26.130 | 1.00 | 63.57 | A |
| ATOM | 11 | CB | ASP | 117 | - 5 | .711 | -14.402 | 27.539 | 1.00 | 63.36 | Ą |
| ATOM | 12 | CG | ASP | 117 | | | -15.163 | | 1.00 | 63.71 | A |
| ATOM | 13 | OD1 | ASP | 117 | - 6 | .090 | -16.247 | 28.965 | 1.00 | 63.24 | A |
| ATOM | 14 | OD2 | ASP | 117 | | | -14.668 | 28.987 | 1.00 | 63.29 | A |
| ATOM | 15 | C | ASP | 117 | - 5 | .651 | -13.585 | 25.184 | 1.00 | 63.31 | A |
| ATOM | 16 | 0 | ASP | 117 | - 6 | .039 | -12.427 | 25.145 | 1.00 | 63.35 | A |
| ATOM | 17 | N | GLN | 118 | -4 | .713 | -14.090 | 24.379 | 1.00 | 62.72 | A |
| ATOM | 18 | H | GLN | 118 | -4 | .450 | -15.040 | 24.541 | 1.00 | 15.00 | A |
| ATOM | 19 | CA | GLN | 118 | -4 | .097 | -13.313 | 23.281 | 1.00 | 61.79 | A |
| ATOM | 20 | CB | GLN | 118 | - 2 | .918 | -14.117 | 22.687 | 1.00 | 62.46 | A |
| ATOM | 21 | CG | GLN | 118 | - 3 | .047 | -15.659 | 22.562 | 1.00 | 62.95 | A |
| ATOM | 22 | CD | GLN | 118 | - 4 | . 277 | -16.118 | 21.790 | | 63.26 | A |
| ATOM | 23 | OE1 | GLN | 118 | - 5 | .396 | -16.000 | 22.277 | 1.00 | 63.43 | A |
| ATOM | 24 | NE2 | GLN | 118 | | | -16.665 | 20.601 | 1.00 | 63.42 | A |
| ATOM | 25 | HE21 | GLN | 118 | -4 | | -16.715 | 19.975 | 1.00 | 15.00 | A |
| ATOM | 26 | HE22 | GLN | 118 | | | -16.995 | 20.298 | 1.00 | 15.00 | A |
| ATOM | 27 | C | GLN | 118 | | | -12.841 | 22.128 | 1.00 | 60.59 | A |
| ATOM | 28 | 0 | GLN | 118 | | | -13.379 | 21.052 | 1.00 | 60.79 | A |
| ATOM | 29 | N | ASN | 119 | | .912 | -11.901 | 22.445 | 1.00 | 58.61 | · A |
| ATOM | 30 | H | ASN | 119 | | | -11.600 | 23.389 | 1.00 | 15.00 | A |
| ATOM | 31 | CA | ASN | 119 | | | -11.222 | 21.386 | | 56.39 | A |
| ATOM | 32 | CB | asn | 119 | | | -11.982 | 20.936 | | 56.95 | A |
| MOTA | 33 | CG | ASN | 119 | | | -13.352 | 20.375 | | 57.45 | A |
| ATOM | 34 | OD1 | | 119 | | .941 | -14.303 | 21.084 | 1.00 | 58.50 | A |
| ATOM | 35 | ND2 | | 119 | | .005 | -13.431 | 19.241 | | 58.58 | A |
| ATOM | 36 | HD21 | | 119 | | .843 | -12.617 | 18.646 | | 15.00 | A |
| MOTA | 37 | HD22 | ASN | 119 | | .740 | -14.221 | 18.684 | | 15.00 | A |
| ATOM | 38 | C | ASN | 119 | | .053 | -9.724 | 21.571 | | 53.62 | A |
| ATCM | 39 | 0 | ASN | 119 | | .,746 | -8.933 | 20.694 | | 56.55 | A |
| ATOM | 40 | N | PRO | 120 | | . 737 | -9.288 | 22.698 | | 50.17 | A |
| ATOM | 41 | CD | PRO | 120 | | .151 | -10.129 | 23.810 | | 51.90 | Ą |
| ATOM | 42 | CA | PRO | 120 | | .402 | -7.945 | 22.818 | | 48.19 | A |
| ATOM | 43 | CB | PRO | 120 | | .191 | -8.008 | 24.117 | | 47.42 | A |
| ATOM | 44 | CG | PRO | 120 | | .444 | -9.493 | 24.321 | | 51.93 | A |
| ATOM | 45 | C | PRJ | 120 | | . 750 | -6.524 | 22.657 | | 45.59 | A |
| ATOM | 46 | 0 | PRO | 120 | | .187 | -5.516 | 23.225 | | 45.37 | A |
| ATOM | 47 | N | GLN | 121 | | .789 | -6.458 | 21.721 | | 38.52 | A |
| ATOM | 48 | Н | GLN | 121 | | . 287 | -7.704 | 21.505 | | 15.00 | A |
| ATOM | 49 | CA | GLN | 121 | | .733 | -5.359 | 20.753 | | 29.14 | A |
| ATOM | 50 | CB | GLN | 121 | | .454 | -5.735 | 19.971 | | 26.30 | A |
| ATOM | 51 | CG | GLN | 121 | | .128 | -4.943 | 18.710 | | 26.84 | A |
| ATOM | 52 | CD | GLN | 121 | | .923 | -3.460 | 18.949 | | 27.26 | A |
| ATOM | 53 | OE1 | GLN | 121 | | .822 | -2.668 | 18.709 | | 28.66 | A |
| ATOM | 54 | NE2 | GLN | 121 | | .717 | -3.100 | 19.341 19.564 | | 33.90 | A |
| ATOM | 56 | | GLN | 121 | | .883 | -3.614 -2.138 | | | 15.00 | A |
| ATOM | 57 | HE22 C | GLN GLN | 121 121 | | .442 | -5.218 | 19.204 19.903 | | 15.00 | A |
| ATOM ATOM | 58 | 0 | GLN | 121 | | .905 | -6.097 | 19.903 | | 26.33 21.41 | A A |
| | 59 | Ŋ | ILE | 122 | | . 288 | -4.051 | 19.834 | | | A |
| ATCM | コブ | 1.4 | | -44 | - 8 | . 205 | -4.031 | 13.414 | 1.00 | 21.21 | A |

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FIGURE 17B

| | | | | • | | _ | | |
|------|-----------|----------|------|-----|--------------------|------------------|------------------|-------------------------|
| 1704 | 60 | н | ILE | 122 | -7.600 | -3.320 | 19.337 | 1.00 15.00 |
| ATOM | 60 | | ILE. | 122 | -9.383 | -3.952 | 18.295 | 1.00 20.92 |
| ATOM | 51 | CA CB | ILE. | 122 | -10.238 | -2.629 | 18.396 | 1.00 22.17 |
| ATOM | 62 | | | 122 | -11.275 | -2.428 | 17.272 | 1.00 21.61 |
| ATOM | 63 | CG2 | ILE | | -11.076 | -2.744 | 19.668 | 1.00 24.13 |
| ATOM | 64 | CG1 | ILE | 122 | | | 20.073 | 1.00 23.04 |
| ATOM | 65 | CD1 | ILE | 122 | -11.751 | -1.440 | | 1.00 18.96 |
| ATOM | 66 | C | ILE | 122 | -8.833 | -4.108 | 16.895 | 1.00 17.93 |
| ATOM | 67 | 0 | ILE | 122 | -8.135 | -3.243 | 16.379 | 1.00 17.93 |
| ATOM | 68 | N | ALA | 123 | -9.159 | -5.240 | 16.283 16.805 | 1.00 14.72 |
| ATOM | 69 | H | ALA | 123 | -9.599 | -5.978 | | 1.00 14.29 |
| ATOM | 70 | CA | ALA | 123 | -8.656 -7.176 | -5.401 -5.868 | 14.917 14.903 | 1.00 14.29 |
| MOTA | 71 | CB | ALA | 123 | | | 13.985 | 1.00 12.83 |
| ATOM | 72 | C | ALA | 123 | -9.483 | -6.315 | 14.323 | 1.00 13.58 |
| ATOM | 73 | 0 | ALA | 123 | -10.170 | -7.261 | 12.724 | 1.00 13.35 |
| ATOM | 74 | N | ALA | 124 | -9.388 | -6.009 | 12.724 | 1.00 15.00 |
| ATOM | 75 | H | ALA | 124 | -8.894 | -5.185 | 12.436 | 1.00 14.55 |
| ATOM | 76 | CA | ALA | 124 | -10.087 | -6.920 | | 1.00 14.33 |
| ATOM | 77 | CB | ALA | 124 | -11.486 | -6.368 | 11.446 10.563 | 1.00 13.54 |
| ATOM | 78 | C | ALA | 124 | -9.271 | -7.123 | 10.363 | 1.00 15.34 |
| MOTA | 79 | 0 | ALA | 124 | -8.501 | -6.274 | 9.937 | 1.00 15.29 |
| MOTA | 80 | N | HIS | 125 | -9.544 | -8.248 | | 1.00 11.49 |
| ATOM | 81 | H | HIS | 125 | -10.100 | -8.900 | 10.426 | 1.00 13.00 |
| ATOM | 82 | CA | HIS | 125 | -9.100 | -8.524 | 8.590 | |
| MOTA | 83 | CB | HIS | 125 | -7.605 | -8.908 | 8.614 | 1.00 11.43 1.00 7.41 |
| ATOM | 84 | CG | HIS | 125 | -7.119 | -9.116 | 7.205 | 1.00 7.41 1.00 6.60 |
| ATOM | 85 | ND1 | | 125 | -6.750 | -8.130 | 6.421 | 1.00 15.00 |
| ATOM | 86 | HD1 | | 125 | -6.708 | -7.168 | 6.621 | |
| ATOM | 87 | CD2 | | 125 | | -10.291 | 6.456 | 1.00 12.36 |
| ATOM | 88 | NE2 | | 125 | -6.670 | -9.971 | 5.234 | 1.00 6.20 |
| ATOM | 89 | CEl | | 125 | -6.462 | -8.646 | 5.211 | 1.00 4.48 1.00 12.63 |
| MOTA | 90 | C | HIS | 125 | -10.024 | -9.570 | 7.931 | 1.00 12.03 |
| ATOM | 91 | 0 | HIS | 125 | -10.324 | | 8.383 | 1.00 15.65 |
| ATOM | 92 | N | VAL | 126 | -10.550 | -9.129 | 6.806 | 1.00 15.00 |
| ATOM | 93 | Н | VAL | 126 | -10.169 | -8.286 | 6.428 6.201 | 1.00 14.38 |
| MOTA | 94 | CA | VAL | 126 | -11.743 | -9.717 | | 1.00 14.38 |
| MOTA | 95 | CB | VAL | 126 | -12.977 | -8.808 | 6.675 7.379 | 1.00 13.37 |
| MOTA | 96 | CG1 | VAL | 126 | -13.794 | -9.722 | 5.814 | 1.00 12.60 |
| MOTA | 97 | CG2 | VAL | 126 | -13.449 | -7.663 | 4.685 | 1.00 16.03 |
| ATOM | 98 | Ċ | VAL | 126 | -11.502 | -9.971 | 4.074 | 1.00 16.42 |
| ATOM | 99 | 0 | VAL | 126 | -10.684 | -9.297 | | 1.00 15.42 |
| ATOM | 100 | N | ILE | 127 | -12.118 | -11.013 | 4.136 4.691 | 1.00 15.00 |
| ATOM | 101 | H | ILE | 127 | -12.807 | -11.532 | 2.831 | 1.00 14.86 |
| ATOM | 102 | CA | ILE | 127 | -11.651 -11.414 | | 3.002 | 1.00 17.56 |
| ATOM | 103 | CB | ILE | 127 | -11.414 | | 1.765 | |
| ATOM | 104 | | ILE | 127 | | -13.316 | 3.399 | 1.00 16.47 |
| ATOM | 105 | | ILE | 127 | | -12.992 | 4.864 | 1.00 19.64 |
| ATOM | 106 | CD1 | ILE | 127 | | -11.269 | 1.765 | 1.00 18.96 |
| ATOM | 107 | C | ILE | 127 | | -11.209 | 2.016 | 1.00 20.01 |
| ATOM | 108 | 0 | ILE | 127 | | -10.882 | 0.581 | 1,00 17.54 |
| ATOM | 109 | N | SER | 128 | | -10.871 | 0.382 | 1.00 15.00 |
| MCTA | 110 | H | SER | 128 | | -10.667 | -0.437 | 1.00 15.55 |
| ATOM | 111 | CA | SER | 128 | | -10.007 | -1.706 | 1.00 18.16 |
| ATOM | 112 | CB | SER | 128 | | -10.130 | -2.574 | 1.00 19.90 |
| ATOM | 113 | ာင္ | SER | 128 | - 12.205 | -11.207 | -2.029 | 1.00 15.00 |
| ATOM | 114 | HG | SER | 128 | | -11.761 | -0.792 | 1.00 13.62 |
| ATOM | 115 | C | SER | 128 | | -12.960 | -0.832 | 1.00 8.98 |
| ATCM | 116 | 0 | SER | 128 | | -11.246 | -1.027 | 1.00 13.36 |
| ATOM | 117 | N | GLU | 129 | | -10.257 | | 1.00 15.00 |
| ATOM | 118 | H | GLU | 129 | | -10.237 | -1.840 | 1.00 17.20 |
| ATOM | 119 | CA | SLU | 129 | - 10.3/3 | 12.024 | | |

FIGURE 17C

| ATOM 120 CB GLU 129 -77.052 -13.117 -1.021 1.00 20.55 ATOM 121 CG GLU 129 -88.092 -12.694 -0.036 1.00 17.92 ATOM 122 CD GLU 129 -88.781 -13.951 0.376 1.00 17.92 ATOM 123 0E1 GLU 129 -19.997 -13.932 0.368 1.00 32.198 ATOM 124 0E2 GLU 129 -18.150 -14.938 0.734 1.00 33.12 ATOM 125 C GLU 129 -17.371 -11.409 -2.809 1.00 17.71 ATOM 126 O GLU 129 -17.371 -11.409 -2.809 1.00 17.71 ATOM 127 N ALA 130 -17.550 -12.145 -3.914 1.00 20.52 ATOM 128 H ALA 130 -17.550 -12.145 -3.914 1.00 20.52 ATOM 129 CA ALA 130 -17.136 -13.057 -3.923 1.00 15.00 ATOM 130 CB ALA 130 -18.279 -11.649 -5.019 1.00 23.36 ATOM 131 C ALA 130 -18.424 -12.633 -6.208 1.00 19.66 ATOM 131 C ALA 130 -19.811 -11.298 -4.570 1.00 29.40 ATOM 132 O ALA 130 -20.519 -12.022 -3.869 1.00 29.40 ATOM 133 N SER 131 -20.198 -10.086 -4.968 1.00 15.00 ATOM 136 CB SER 131 -20.198 -10.086 -4.968 1.00 15.00 ATOM 137 CG SER 131 -21.892 -9.782 -4.732 1.00 20.04 ATOM 138 H SER 131 -21.892 -9.782 -4.732 1.00 20.04 ATOM 139 C SER 131 -22.236 -10.653 -4.732 1.00 20.04 ATOM 130 C SER 131 -22.326 -10.653 -4.732 1.00 20.05 ATOM 140 O SER 131 -22.326 -10.051 -5.668 1.00 17.15 ATOM 141 N SER 132 -23.326 -10.531 -5.868 1.00 17.15 ATOM 140 C SER 131 -22.326 -10.501 -5.688 1.00 17.15 ATOM 141 N SER 132 -23.367 -10.653 -6.786 1.00 15.00 ATOM 142 H SER 132 -23.367 -10.653 -6.786 1.00 15.00 ATOM 144 CB SER 131 -22.546 -10.501 -5.688 1.00 17.15 ATOM 144 CB SER 132 -23.566 -12.516 -5.889 1.00 15.00 ATOM 145 CG SER 131 -22.546 -10.501 -5.688 1.00 17.15 ATOM 140 N SER 132 -23.566 -10.531 -5.868 1.00 17.15 ATOM 141 N SER 132 -23.367 -10.853 -6.786 1.00 15.00 ATOM 142 H SER 132 -23.566 -10.531 -5.889 1.00 15.00 ATOM 144 CB SER 132 -23.566 -10.531 -5.889 1.00 15.00 ATOM 145 CG SER 131 -22.566 -10.501 -1.944 -4.179 1.00 20.07 ATOM 146 N SER 132 -26.506 -20.651 -1.00 20.07 ATOM 147 C SER 132 -26.506 -20.651 -20.940 -20. | | | | | | |
|--|-------|-----|--------|-----|-------|---|
| ATOM 121 CG GLU 129 -18.092 -12.694 -0.036 1.00 17.92 ATOM 122 CD GLU 129 -18.997 -13.992 0.368 1.00 32.199 ATOM 123 OEI GLU 129 -19.997 -13.992 0.368 1.00 32.23 ATOM 124 OEZ GLU 129 -17.371 -11.409 -2.809 1.00 17.15 ATOM 125 C GLU 129 -17.371 -11.409 -2.809 1.00 17.15 ATOM 126 O GLU 129 -17.371 -11.409 -2.809 1.00 17.15 ATOM 126 O GLU 129 -17.371 -11.409 -2.809 1.00 17.15 ATOM 127 N ALA 130 -17.550 -12.145 -3.914 1.00 20.52 ATOM 128 H ALA 130 -17.550 -12.145 -3.914 1.00 20.52 ATOM 128 H ALA 130 -17.550 -12.145 -3.914 1.00 20.52 ATOM 129 CA ALA 130 -18.379 -11.649 -5.019 1.00 23.36 ATOM 130 CB ALA 130 -18.379 -11.649 -5.019 1.00 23.36 ATOM 131 C ALA 130 -19.811 -11.298 -4.570 1.00 26.96 ATOM 131 C ALA 130 -20.519 -12.022 -3.869 1.00 29.40 ATOM 133 N SER 131 -20.198 -10.086 -4.968 1.00 21.70 ATOM 136 CB SER 131 -21.592 -9.762 -4.732 1.00 20.04 ATOM 136 CB SER 131 -21.592 -9.762 -4.732 1.00 20.05 ATOM 137 OG SER 131 -21.592 -9.762 -4.732 1.00 20.05 ATOM 137 OG SER 131 -23.182 -6.001 -4.435 1.00 15.00 ATOM 139 C SER 131 -23.182 -6.001 -4.435 1.00 15.00 ATOM 139 C SER 131 -23.182 -6.001 -4.435 1.00 15.00 ATOM 141 N SER 132 -23.756 -10.501 -5.668 1.00 17.15 ATOM 140 O SER 131 -22.236 -10.853 -6.766 1.00 14.30 ATOM 141 N SER 132 -23.756 -10.501 -5.668 1.00 17.15 ATOM 144 CB SER 132 -23.756 -10.501 -5.668 1.00 17.15 ATOM 147 C SER 132 -23.756 -10.731 -5.187 1.00 20.15 0.00 ATOM 147 C SER 132 -23.756 -10.731 -5.187 1.00 20.15 0.00 ATOM 147 C SER 132 -23.756 -10.731 -5.187 1.00 20.15 0.00 ATOM 149 N LYS 133 -22.566 -2.606 -9.063 -6.181 1.00 21.60 ATOM 147 C SER 132 -23.756 -10.731 -5.187 1.00 20.15 0.00 ATOM 149 N LYS 133 -27.664 -8.364 -4.299 1.00 15.00 20.77 ATOM 149 N LYS 133 -27.664 -8.364 -4.354 1.00 21.160 ATOM 150 C LYS 133 -27.664 -8.364 -4.354 1.00 21.160 ATOM 150 C LYS 133 -27.664 -8.364 -4.760 1.00 21.50 0.00 ATOM 150 C LYS 133 -27.684 -8.364 -4.760 1.00 21.50 0.00 ATOM 150 C LYS 133 -27.684 -8.364 -4.760 1.00 21.50 0.00 ATOM 150 C LYS 133 -27.555 -6.876 -7.7551 -0.288 1.00 21.50 0.00 ATOM 150 C LYS 133 -27.5 | A TOM | 120 | CB | GLU | 129 | |
| ATOM 123 OEL GLU 129 | | | | | | |
| ATOM 123 OEL GLU 129 -19.997 -13.932 0.368 1.00 32.23 ATOM 124 OEZ GLU 129 -18.150 -14.938 0.734 1.00 33.12 ATOM 125 C GLU 129 -17.371 -11.409 -2.809 1.00 17.71 ATOM 126 O GLU 129 -17.371 -11.409 -2.809 1.00 17.71 ATOM 127 N ALA 130 -17.550 -12.145 -3.914 1.00 20.52 ATOM 128 H ALA 130 -17.136 -13.057 -3.923 1.00 15.00 ATOM 129 CA ALA 130 -18.379 -11.649 -5.019 1.00 23.36 ATOM 130 CB ALA 130 -18.479 -11.649 -5.019 1.00 23.36 ATOM 131 C ALA 130 -19.811 -11.298 -4.570 1.00 26.96 ATOM 132 O ALA 130 -20.519 -10.066 -4.968 1.00 29.40 ATOM 133 N SER 131 -20.198 -10.066 -4.968 1.00 21.70 ATOM 134 H SER 131 -21.592 -9.762 -4.732 1.00 20.04 ATOM 135 CA SER 131 -21.592 -9.762 -4.732 1.00 20.04 ATOM 136 CB SER 131 -21.829 -8.266 -4.787 1.00 20.65 ATOM 137 OG SER 131 -23.329 -70.099 -4.559 1.00 20.04 ATOM 138 HG SER 131 -23.329 -70.099 -4.559 1.00 15.20 ATOM 139 C SER 131 -22.366 -10.651 -4.455 1.00 15.24 ATOM 130 C SER 131 -22.366 -10.651 -5.668 1.00 17.15 ATOM 140 O SER 131 -22.236 -10.853 -6.786 1.00 15.24 ATOM 140 C SER 131 -22.236 -10.853 -6.786 1.00 15.02 ATOM 141 N SER 132 -23.756 -10.731 -5.187 1.00 20.15 ATOM 144 CB SER 132 -23.967 -10.596 -4.209 1.00 15.00 ATOM 145 OG SER 132 -26.016 -12.944 -4.179 1.00 15.00 ATOM 146 HG SER 132 -26.016 -12.944 -4.179 1.00 15.00 ATOM 147 C SER 132 -26.016 -12.944 -4.179 1.00 15.00 ATOM 148 O SER 132 -26.016 -12.944 -4.179 1.00 15.00 ATOM 150 H LYS 133 -25.606 -9.06 -6.751 1.00 20.77 ATOM 150 H LYS 133 -27.004 -7.309 5.256 1.00 2.162 ATOM 150 H LYS 133 -27.004 -7.309 5.256 1.00 2.167 ATOM 150 H LYS 133 -27.004 -7.309 5.256 1.00 2.167 ATOM 150 H LYS 133 -27.004 -7.309 5.256 1.00 2.107 ATOM 150 H LYS 133 -27.004 -7.309 5.256 1.00 2.107 ATOM 150 H LYS 133 -27.004 -7.309 5.256 1.00 2.107 ATOM 150 H LYS 133 -27.004 -7.309 5.256 1.00 2.107 ATOM 150 H LYS 133 -27.004 -7.309 5.256 1.00 2.107 ATOM 150 C THR 134 -26.200 -6.052 -7.983 1.00 2.107 ATOM 150 H LYS 133 -27.004 -7.309 5.256 1.00 2.107 ATOM 150 H LYS 133 -27.004 -7.309 5.256 1.00 2.107 ATOM 150 H LYS 133 -27.004 -7.309 5.256 1.00 2. | | | | | | |
| ATOM 124 OEZ GLU 129 18.150 14.938 0.734 1.00 33.12 ATOM 125 C GLU 129 17.771 -11.499 -2.809 1.00 17.71 ATOM 126 O GLU 129 17.972 -10.389 2.553 1.00 21.59 ATOM 127 N ALA 130 17.550 -12.145 -3.914 1.00 20.52 ATOM 128 H ALA 130 17.136 -13.057 -3.923 1.00 15.00 ATOM 129 CA ALA 130 17.136 -13.057 -3.923 1.00 15.00 ATOM 129 CA ALA 130 -18.424 -12.633 -6.208 1.00 19.56 ATOM 130 CB ALA 130 -18.424 -12.633 -6.208 1.00 19.56 ATOM 131 C ALA 130 -18.424 -12.633 -6.208 1.00 19.56 ATOM 132 C ALA 130 -19.811 -11.298 -4.570 1.00 26.86 ATOM 133 C SER 131 -20.5198 10.066 -4.968 1.00 29.40 ATOM 134 H SER 131 -20.519 -12.022 -3.869 1.00 29.40 ATOM 135 CA SER 131 -21.829 -9.481 5.410 1.00 15.00 ATOM 136 CB SER 131 -21.829 -9.782 -4.732 1.00 20.04 ATOM 136 CB SER 131 -21.829 -9.2782 -4.732 1.00 20.04 ATOM 137 OG SER 131 -23.129 -7.069 -4.559 1.00 15.24 ATOM 137 OG SER 131 -23.129 -7.069 -4.559 1.00 15.24 ATOM 137 OG SER 131 -23.129 -7.069 -4.559 1.00 15.24 ATOM 137 OG SER 131 -22.236 -10.853 6.786 1.00 17.15 ATOM 140 O SER 131 -22.236 -10.853 6.786 1.00 17.15 ATOM 141 N SER 132 -23.967 -10.566 4.209 1.00 15.00 ATOM 141 N SER 132 -23.967 -10.566 4.209 1.00 15.00 ATOM 144 CB SER 132 -23.967 -10.566 4.209 1.00 15.00 ATOM 144 CB SER 132 -23.967 -10.566 4.209 1.00 15.00 ATOM 144 CB SER 132 -25.266 -12.616 -5.893 1.00 16.00 ATOM 147 C SER 132 -25.266 -12.616 -5.893 1.00 16.00 ATOM 147 C SER 132 -26.501 12.244 4.179 1.00 20.15 ATOM 147 C SER 132 -26.501 12.244 4.179 1.00 20.15 ATOM 147 C SER 132 -26.501 12.244 4.179 1.00 20.15 .00 ATOM 147 C SER 132 -26.501 12.244 4.179 1.00 20.15 .00 ATOM 147 C SER 132 -26.501 12.244 4.179 1.00 15.00 ATOM 147 C SER 132 -26.501 12.244 4.179 1.00 15.00 ATOM 147 C SER 132 -26.501 12.244 4.179 1.00 15.00 ATOM 147 C SER 132 -26.501 12.244 4.179 1.00 15.00 ATOM 147 C SER 132 -26.501 12.244 4.179 1.00 15.00 ATOM 147 C SER 132 -26.501 12.244 4.179 1.00 15.00 ATOM 147 C SER 132 -26.501 12.244 4.179 1.00 15.00 ATOM 147 C SER 132 -26.501 12.244 4.10 12.28 1.60 SER 133 -27.64 6.80 -27.98 1.00 12.50 ATOM 147 C SER 13 | | | | | | |
| ATOM 125 C CLU 129 -17.371 -11.409 -2.809 1.00 17.71 ATOM 126 O GLU 129 -17.371 -11.409 -2.809 1.00 17.71 ATOM 126 O GLU 129 -17.550 -12.145 -3.914 1.00 20.52 ATOM 127 N ALA 130 -17.550 -12.145 -3.914 1.00 20.52 ATOM 128 H ALA 130 -17.550 -12.145 -3.914 1.00 20.52 ATOM 129 CA ALA 130 -17.136 -13.057 -3.923 1.00 15.00 ATOM 130 CB ALA 130 -18.424 -12.633 -6.208 1.00 19.66 ATOM 131 C ALA 130 -19.811 -11.298 -4.570 1.00 26.86 ATOM 131 C ALA 130 -19.811 -11.298 -4.570 1.00 26.86 ATOM 132 O ALA 130 -20.519 -12.022 -3.869 1.00 29.40 ATOM 133 N SER 131 -20.198 -10.086 4.968 1.00 29.40 ATOM 134 H SER 131 -20.198 -10.086 4.968 1.00 29.40 ATOM 135 CA SER 131 -21.899 -8.266 -4.782 1.00 15.00 ATOM 136 CB SER 131 -21.899 -8.266 -4.782 1.00 20.04 ATOM 136 CB SER 131 -21.899 -8.266 -4.782 1.00 20.05 ATOM 137 OG SER 131 -23.329 -7.069 -4.559 1.00 15.20 ATOM 139 C SER 131 -23.329 -7.069 -4.559 1.00 15.20 ATOM 130 N SER 131 -22.236 -10.853 -6.786 1.00 17.15 ATOM 140 O SER 131 -22.236 -10.853 -6.786 1.00 17.15 ATOM 140 N SER 132 -23.967 -10.586 -4.209 1.00 17.15 ATOM 141 N SER 132 -23.967 -10.586 -4.209 1.00 17.15 ATOM 144 CB SER 132 -23.967 -10.586 -4.209 1.00 17.15 ATOM 146 HG SER 132 -25.266 -12.616 -5.893 1.00 12.02 ATOM 147 C SER 132 -25.266 -12.616 -5.893 1.00 12.02 ATOM 148 O SER 132 -26.03 -12.324 -4.894 1.00 20.384 ATOM 147 C SER 132 -26.535 -10.544 -7.547 1.00 20.27 ATOM 148 O SER 132 -26.535 -10.544 -7.547 1.00 20.27 ATOM 148 O SER 132 -26.535 -10.544 -7.547 1.00 20.39 ATOM 150 H LYS 133 -27.606 -9.063 -6.118 1.00 21.87 ATOM 150 H LYS 133 -27.606 -9.063 -6.118 1.00 21.87 ATOM 150 H LYS 133 -27.606 -9.063 -6.118 1.00 21.87 ATOM 150 H LYS 133 -27.606 -9.063 -6.118 1.00 21.87 ATOM 150 H LYS 133 -27.606 -9.063 -6.118 1.00 21.87 ATOM 150 H LYS 133 -27.724 -8.110 -4.359 1.00 15.00 ATOM 150 H LYS 133 -27.606 -9.063 -6.118 1.00 21.97 ATOM 150 H LYS 133 -27.606 -9.063 -6.118 1.00 21.97 ATOM 150 H LYS 133 -27.606 -9.063 -6.118 1.00 21.97 ATOM 150 H LYS 133 -27.606 -9.063 -6.118 1.00 21.97 ATOM 150 H LYS 133 -27.606 -9.063 -6.118 | | | | | | — · · · · · · · · · · · · · · · · · · · |
| ATOM 126 O GLU 129 -17.972 -10.389 -2.553 1.00 21.59 ATOM 127 N ALIA 130 -17.550 -12.145 -3.914 1.00 20.52 ATOM 128 H ALIA 130 -17.136 -13.057 -3.923 1.00 15.00 ATOM 129 CA ALIA 130 -18.179 -11.649 -5.019 1.00 13.66 ATOM 131 C ALIA 130 -18.179 -11.649 -5.019 1.00 13.66 ATOM 131 C ALIA 130 -18.179 -11.649 -6.208 1.00 19.66 ATOM 131 C ALIA 130 -20.519 -12.022 -3.669 1.00 29.40 ATOM 132 O ALIA 130 -20.519 -12.022 -3.669 1.00 29.40 ATOM 133 N SER 131 -20.198 -10.086 -4.968 1.00 29.40 ATOM 134 H SER 131 -19.515 -9.481 -5.410 1.00 15.00 ATOM 135 CA SER 131 -21.592 -9.782 -4.732 1.00 20.65 ATOM 136 CB SER 131 -21.592 -9.782 -4.732 1.00 20.65 ATOM 137 OG SER 131 -21.592 -9.782 -4.732 1.00 20.65 ATOM 139 C SER 131 -23.182 -8.001 -4.435 1.00 15.00 ATOM 139 C SER 131 -22.546 -10.501 -5.668 1.00 17.15 ATOM 140 O SER 131 -22.546 -10.501 -5.668 1.00 17.15 ATOM 141 N SER 132 -23.756 -10.731 -5.187 1.00 20.15 ATOM 141 N SER 132 -23.967 -10.585 -4.09 1.00 14.30 ATOM 144 CB SER 132 -23.967 -10.586 -4.209 1.00 14.30 ATOM 144 CB SER 132 -23.967 -10.586 -4.209 1.00 15.00 ATOM 145 OG SER 132 -23.967 -10.586 -4.209 1.00 15.00 ATOM 146 BG SER 132 -25.666 -12.616 -5.893 1.00 15.00 ATOM 147 C SER 132 -25.727 -10.268 -6.671 1.00 20.75 ATOM 146 BG SER 132 -26.203 -12.344 -4.894 1.00 23.84 ATOM 146 BG SER 132 -26.506 -9.063 -6.118 1.00 20.75 ATOM 148 O SER 132 -26.506 -9.063 -6.118 1.00 20.77 ATOM 148 O SER 132 -26.506 -9.063 -6.118 1.00 20.27 ATOM 148 O SER 132 -26.606 -17.916 -6.517 1.00 20.27 ATOM 148 O SER 132 -26.606 -9.063 -6.118 1.00 20.27 ATOM 148 O SER 132 -26.606 -9.063 -6.118 1.00 20.27 ATOM 150 A LYS 133 -26.606 -9.063 -6.118 1.00 20.27 ATOM 150 A LYS 133 -26.606 -9.063 -6.118 1.00 20.27 ATOM 150 A LYS 133 -26.606 -9.063 -6.118 1.00 20.27 ATOM 150 C LYS 133 -27.024 -7.309 -9.5256 1.00 15.00 ATOM 150 C LYS 133 -27.024 -7.309 -9.5256 1.00 20.27 ATOM 150 C LYS 133 -27.024 -7.309 -9.5256 1.00 20.27 ATOM 150 C LYS 133 -27.024 -7.309 -9.5256 1.00 20.27 ATOM 150 C LYS 133 -27.024 -7.309 -9.5256 1.00 20.27 ATOM 160 C LYS 133 -27.024 -7 | | | | | | |
| ATOM 127 N ALA 130 | | | | | | |
| ATOM 128 H ALA 130 | | | | | | |
| ATOM 129 CA ALA 130 | | | | | | |
| ATOM 130 CB ALA 130 | MOTA | _ | | | | |
| ATOM 131 C ALA 130 | | | | | | 20.0.0 |
| ATOM 133 N SER 131 -20.519 -12.022 -3.869 1.00 29.40 ATOM 133 N SER 131 -20.198 -10.086 -4.968 1.00 21.70 ATOM 134 H SER 131 -19.515 -9.481 -5.410 1.00 21.70 ATOM 135 CA SER 231 -21.592 -9.782 -4.732 1.00 20.04 ATOM 136 CB SER 131 -21.592 -9.782 -4.732 1.00 20.04 ATOM 137 OG SER 131 -23.182 -8.266 -4.787 1.00 20.65 ATOM 138 HG SER 131 -23.182 -8.001 -4.435 1.00 15.00 ATOM 139 C SER 131 -22.546 -10.501 -5.668 1.00 17.15 ATOM 140 O SER 131 -22.546 -10.501 -5.668 1.00 17.15 ATOM 141 N SER 132 -23.756 -10.731 -5.187 1.00 20.15 ATOM 142 H SER 132 -23.967 -10.586 -4.299 1.00 15.00 ATOM 144 CB SER 132 -24.674 -11.250 -6.218 1.00 15.00 ATOM 145 CB SER 132 -24.674 -11.250 -6.218 1.00 15.00 ATOM 146 MG SER 132 -26.203 -12.324 -4.894 1.00 23.84 ATOM 147 C SER 132 -26.203 -12.324 -4.894 1.00 23.84 ATOM 148 O SER 132 -26.516 -12.944 -4.179 1.00 15.00 ATOM 149 N LYS 133 -24.904 -8.969 -5.397 1.00 20.07 ATOM 149 N LYS 133 -24.904 -8.969 -5.397 1.00 20.07 ATOM 150 H LYS 133 -24.904 -8.969 -5.397 1.00 20.27 ATOM 151 CA LYS 133 -27.024 -7.309 -5.256 1.10 0.21.67 ATOM 154 CD LYS 133 -27.684 -8.364 -4.354 1.00 21.67 ATOM 155 CE LYS 133 -27.024 -7.309 -5.256 1.00 23.08 ATOM 156 N LYS 133 -27.024 -7.309 -5.256 1.00 23.08 ATOM 157 KB LYS 133 -27.684 -8.364 -4.354 1.00 21.07 ATOM 158 LYS 133 -31.862 -7.351 -6.218 1.00 15.00 ATOM 159 HZ LYS 133 -31.323 -7.515 -5.345 1.00 21.56 ATOM 156 N LYS 133 -31.323 -7.515 -5.345 1.00 21.56 ATOM 157 KB LYS 133 -31.323 -7.551 -6.218 1.00 22.95 ATOM 160 C LYS 133 -31.333 -6.654 -4.760 1.00 27.36 ATOM 158 C LYS 133 -31.333 -6.654 -4.760 1.00 27.36 ATOM 161 O LYS 133 -24.394 -8.364 -4.750 1.00 27.36 ATOM 160 C LYS 133 -31.327 -7.351 -6.218 1.00 15.00 ATOM 161 O LYS 133 -3.155 -8.299 -7.884 -5.670 1.00 27.36 ATOM 160 C LYS 133 -31.333 -6.654 -4.760 1.00 15.00 ATOM 161 O LYS 133 -3.155 -8.299 -7.881 -5.345 1.00 21.56 ATOM 161 O LYS 133 -24.398 -6.801 -7.097 1.00 17.94 ATOM 161 O LYS 133 -3.155 -8.299 -7.885 1.00 22.95 ATOM 161 O LYS 133 -24.398 -6.801 -7.097 1.00 22.95 ATOM 163 HR THR 134 -26.540 -7.397 | MOTA | | | | | |
| ATOM 133 N SER 131 -20.198 -10.086 -4.968 1.00 21.70 ATOM 134 H SER 131 -19.515 -9.481 -5.410 1.00 15.00 ATOM 135 CA SER 131 -21.592 -9.782 -4.732 1.00 20.04 ATOM 136 CB SER 131 -21.592 -9.782 -4.732 1.00 20.04 ATOM 137 OG SER 131 -21.829 -8.266 -4.787 1.00 20.65 ATOM 138 HG SER 131 -23.182 -8.001 -4.435 1.00 15.00 ATOM 138 HG SER 131 -23.182 -8.001 -4.435 1.00 15.00 ATOM 139 C SER 131 -22.546 -10.501 -5.668 1.00 17.15 ATOM 140 O SER 131 -22.546 -10.501 -5.668 1.00 17.15 ATOM 141 N SER 132 -23.756 -10.731 -5.187 1.00 20.15 ATOM 142 H SER 132 -23.756 -10.731 -5.187 1.00 20.15 ATOM 143 CA SER 132 -24.674 -11.250 -6.218 1.00 21.62 ATOM 144 CB SER 132 -26.203 -12.324 -4.894 1.00 23.84 ATOM 146 HG SER 132 -26.016 -12.944 -4.179 1.00 15.00 ATOM 147 C SER 132 -25.727 -10.268 -6.671 1.00 20.07 ATOM 148 O SER 132 -25.526 -9.063 -6.118 1.00 21.87 ATOM 149 N LYS 133 -25.606 -9.063 -6.118 1.00 21.87 ATOM 150 H LYS 133 -24.904 -8.969 -5.397 1.00 15.00 ATOM 151 CA LYS 133 -27.684 -8.364 -4.354 1.00 21.87 ATOM 150 C LYS 133 -27.684 -8.364 -4.354 1.00 21.87 ATOM 155 CE LYS 133 -27.684 -8.364 -4.354 1.00 27.36 ATOM 156 NZ LYS 133 -27.684 -8.364 -4.354 1.00 21.56 ATOM 158 HZ2 LYS 133 -27.684 -8.364 -4.354 1.00 21.56 ATOM 156 NZ LYS 133 -27.684 -8.364 -4.354 1.00 21.57 ATOM 156 NZ LYS 133 -27.684 -8.364 -4.354 1.00 21.50 ATOM 157 HZ1 LYS 133 -27.684 -8.364 -4.354 1.00 21.50 ATOM 158 HZ2 LYS 133 -27.684 -8.364 -4.354 1.00 21.50 ATOM 158 HZ2 LYS 133 -31.323 -7.515 -5.345 1.00 27.36 ATOM 150 C LYS 133 -27.684 -8.364 -4.750 1.00 27.36 ATOM 150 C LYS 133 -27.684 -8.364 -4.354 1.00 21.50 ATOM 160 C LYS 133 -27.684 -8.364 -4.354 1.00 21.50 ATOM 158 HZ2 LYS 133 -31.323 -7.515 -5.345 1.00 21.56 ATOM 160 C LYS 133 -27.684 -8.364 -4.354 1.00 21.50 ATOM 161 O LYS 133 -27.575 -6.130 -8.99 1.00 15.00 ATOM 160 C LYS 133 -27.575 -6.130 -8.99 1.00 15.00 ATOM 160 C LYS 133 -27.575 -6.00 -7.99 1.00 15.00 ATOM 161 O LYS 133 -27.575 -6.00 -7.99 1.00 24.59 ATOM 162 N THR 134 -26.232 -4.411 -11.456 1.00 15.00 ATOM 163 H THR 134 -26.232 -4.411 -11.456 1 | MOTA | | | | | |
| ATOM 134 H SER 131 -19.515 -9.481 -5.410 1.00 15.00 ATOM 135 CA SER 131 -21.592 -9.782 -4.732 1.00 20.04 ATOM 136 CB SER 131 -21.829 -8.266 -4.787 1.00 20.065 ATOM 137 OG SER 131 -23.182 -8.001 -4.435 1.00 15.24 ATOM 138 HG SER 131 -23.182 -8.001 -4.435 1.00 15.24 ATOM 139 C SER 131 -22.326 -10.853 -6.786 1.00 17.15 ATOM 140 O SER 131 -22.3329 -7.069 -4.559 1.00 15.00 ATOM 141 N SER 132 -22.336 -10.853 -6.786 1.00 17.15 ATOM 142 H SER 132 -23.756 -10.731 -5.187 1.00 20.15 ATOM 144 CB SER 132 -23.967 -10.586 -4.209 1.00 15.00 ATOM 144 CB SER 132 -24.674 -11.250 -6.218 1.00 21.62 ATOM 144 CB SER 132 -25.266 -12.616 -5.893 1.00 16.00 ATOM 146 HG SER 132 -26.203 -12.324 -4.894 1.00 23.84 ATOM 147 C SER 132 -26.016 -12.944 -4.179 1.00 15.00 ATOM 148 O SER 132 -26.535 -10.544 -7.547 1.00 20.07 ATOM 149 N LYS 133 -25.606 -9.063 -6.118 1.00 20.07 ATOM 150 H LYS 133 -25.606 -9.063 -6.118 1.00 21.67 ATOM 151 CA LYS 133 -26.406 -7.916 -6.517 1.00 19.23 ATOM 152 CB LYS 133 -27.024 -8.364 -4.354 1.00 21.07 ATOM 153 CG LYS 133 -27.024 -8.364 -4.354 1.00 21.07 ATOM 155 CL LYS 133 -27.024 -8.364 -4.354 1.00 21.07 ATOM 157 HZ LYS 133 -27.024 -8.364 -4.354 1.00 21.07 ATOM 158 HZ LYS 133 -27.024 -8.364 -4.354 1.00 21.07 ATOM 159 HZ LYS 133 -27.024 -8.364 -4.354 1.00 21.07 ATOM 150 H LYS 133 -27.024 -8.364 -4.354 1.00 21.07 ATOM 150 H LYS 133 -27.024 -8.364 -4.354 1.00 21.07 ATOM 150 H LYS 133 -27.024 -8.364 -4.354 1.00 21.07 ATOM 150 H LYS 133 -27.024 -8.364 -4.354 1.00 21.07 ATOM 150 H LYS 133 -27.024 -8.364 -4.354 1.00 21.07 ATOM 150 H LYS 133 -27.024 -8.364 -4.354 1.00 22.07 ATOM 150 H LYS 133 -27.024 -8.364 -4.354 1.00 22.07 ATOM 150 H LYS 133 -27.024 -8.364 -4.354 1.00 22.07 ATOM 150 H LYS 133 -27.024 -8.364 -4.354 1.00 22.07 ATOM 150 H LYS 133 -27.024 -8.364 -4.354 1.00 22.07 ATOM 150 H LYS 133 -27.024 -8.364 -4.354 1.00 22.07 ATOM 150 H LYS 133 -27.569 -6.579 -0.00 22.07 ATOM 150 H LYS 133 -27.569 -0.00 22.0 | ATOM | 132 | 0 | | | |
| ATOM 135 CA SER 131 -21.592 -9.782 -4.732 1.00 20.04 ATOM 136 CB SER 131 -21.829 -8.266 -4.787 1.00 20.65 ATOM 137 OG SER 131 -23.182 -8.001 -4.435 1.00 15.04 ATOM 138 HG SER 131 -23.182 -8.001 -4.435 1.00 15.00 ATOM 139 C SER 131 -23.182 -8.001 -5.668 1.00 17.15 ATOM 140 O SER 131 -22.546 -10.501 -5.668 1.00 17.15 ATOM 141 N SER 132 -22.546 -10.501 -5.668 1.00 14.30 ATOM 141 N SER 132 -23.756 -10.731 -5.187 1.00 20.15 ATOM 142 H SER 132 -23.756 -10.731 -5.187 1.00 20.15 ATOM 143 CA SER 132 -24.674 -11.250 -6.218 1.00 21.62 ATOM 144 CB SER 132 -25.266 -12.616 -5.893 1.00 15.00 ATOM 145 OG SER 132 -26.203 -12.324 -4.894 1.00 23.84 ATOM 146 HG SER 132 -26.016 12.944 -4.179 1.00 15.00 ATOM 147 C SER 132 -26.503 -12.324 -4.894 1.00 23.84 ATOM 146 HG SER 132 -25.727 -10.268 -6.671 1.00 20.07 ATOM 147 D SER 132 -26.535 -10.544 -7.547 1.00 20.07 ATOM 148 O SER 132 -26.535 -10.544 -7.547 1.00 20.07 ATOM 149 N LYS 133 -24.904 -8.969 -5.397 1.00 15.00 ATOM 150 H LYS 133 -24.904 -8.969 -5.397 1.00 15.00 ATOM 151 CA LYS 133 -27.024 -7.309 -5.256 1.00 23.08 ATOM 152 CB LYS 133 -27.024 -7.309 -5.256 1.00 23.08 ATOM 154 CD LYS 133 -27.024 -7.309 -5.556 1.00 23.08 ATOM 155 CE LYS 133 -27.024 -7.351 -6.218 1.00 21.07 ATOM 158 HZ2 LYS 133 -31.333 -6.654 -4.354 1.00 21.07 ATOM 158 HZ2 LYS 133 -31.333 -6.664 -4.354 1.00 21.07 ATOM 159 HZ3 LYS 133 -31.333 -6.664 -4.354 1.00 21.07 ATOM 159 HZ3 LYS 133 -31.333 -6.664 -4.750 1.00 27.36 ATOM 150 C LYS 133 -27.555 -6.100 23.08 ATOM 151 CA LYS 133 -27.024 -7.309 -5.256 1.00 23.08 ATOM 150 C LYS 133 -27.024 -7.309 -5.256 1.00 23.08 ATOM 151 CA LYS 133 -27.024 -7.309 -5.256 1.00 23.08 ATOM 152 CB LYS 133 -27.024 -7.309 -5.256 1.00 23.08 ATOM 154 CD LYS 133 -27.024 -7.309 -5.256 1.00 23.08 ATOM 157 HZ1 LYS 133 -31.525 -6.665 -7.963 1.00 25.00 ATOM 159 HZ3 LYS 133 -31.525 -6.66 -7.965 1.00 23.08 ATOM 150 C LYS 133 -27.024 -7.309 -5.256 1.00 23.08 ATOM 150 C LYS 133 -27.555 -6.200 1.00 27.36 ATOM 160 C LYS 133 -27.555 -6.200 1.00 27.36 ATOM 160 C LYS 133 -27.555 -6.200 1.00 27.36 ATOM 160 C L | ATOM | 133 | N | | | |
| ATOM 136 CB SER 131 -21.829 -8.266 -4.787 1.00 20.65 ATOM 137 OG SER 131 -23.182 -8.001 -4.435 1.00 15.24 ATOM 138 HG SER 131 -23.329 -7.069 -4.559 1.00 15.00 ATOM 139 C SER 131 -22.546 -10.501 -5.668 1.00 17.15 ATOM 140 O SER 131 -22.236 -10.853 -6.786 1.00 17.15 ATOM 141 N SER 132 -23.756 -10.731 -5.187 1.00 20.15 ATOM 142 H SER 132 -23.967 -10.586 -4.209 1.00 15.00 ATOM 143 CA SER 132 -24.674 -11.250 -6.218 1.00 21.62 ATOM 144 CB SER 132 -24.674 -11.250 -6.228 1.00 21.62 ATOM 145 OG SER 132 -26.206 -12.616 -5.893 1.00 15.00 ATOM 146 HG SER 132 -26.2016 -12.944 -4.179 1.00 16.00 ATOM 147 C SER 132 -26.2016 -12.944 -4.179 1.00 15.00 ATOM 148 O SER 132 -26.5727 -10.268 -6.671 1.00 20.07 ATOM 149 N LYS 133 -25.506 -9.063 -6.18 1.00 21.87 ATOM 150 H LYS 133 -25.506 -9.063 -6.18 1.00 21.87 ATOM 151 CA LYS 133 -24.904 -8.969 -5.397 1.00 15.00 ATOM 152 CB LYS 133 -27.024 -7.309 -5.256 1.00 23.08 ATOM 153 CG LYS 133 -27.024 -8.3164 -4.354 1.00 21.07 ATOM 154 CD LYS 133 -27.024 -8.3164 -4.354 1.00 21.07 ATOM 155 CE LYS 133 -27.024 -8.3164 -4.354 1.00 21.07 ATOM 155 CE LYS 133 -31.862 -7.351 -6.218 1.00 15.00 ATOM 159 HZ3 LYS 133 -31.862 -7.351 -6.218 1.00 15.00 ATOM 150 H LYS 133 -31.862 -7.351 -6.218 1.00 15.00 ATOM 150 H LYS 133 -31.333 -6.654 -4.760 1.00 20.07 ATOM 150 KZ LYS 133 -31.333 -6.654 -4.354 1.00 21.07 ATOM 150 KZ LYS 133 -31.333 -6.654 -4.354 1.00 21.07 ATOM 150 KZ LYS 133 -31.333 -6.654 -4.354 1.00 21.07 ATOM 150 KZ LYS 133 -31.333 -6.654 -4.760 1.00 23.08 ATOM 150 KZ LYS 133 -31.555 -6.218 1.00 15.00 ATOM 160 C LYS 133 -31.333 -6.654 -4.760 1.00 23.056 ATOM 160 C LYS 133 -31.333 -6.654 -4.760 1.00 23.056 ATOM 160 C LYS 133 -31.333 -6.654 -4.760 1.00 23.056 ATOM 160 C LYS 133 -31.333 -6.654 -7.995 1.00 22.97 ATOM 161 N THR 134 -26.260 -6.052 -7.983 1.00 22.95 ATOM 163 K THR 134 -26.260 -6.052 -7.983 1.00 22.95 ATOM 164 CB THR 134 -26.260 -6.052 -7.983 1.00 22.95 ATOM 165 CB THR 134 -26.560 -6.052 -7.983 1.00 22.95 ATOM 165 CB THR 134 -26.560 -6.004 -7.916 -6.00 1.00 15.00 ATOM 163 CB THR 134 -26.560 -6. | ATOM | 134 | | | | |
| ATOM 137 OG SER 131 -23.182 -8.001 -4.435 1.00 15.24 ATOM 138 HG SER 131 -23.329 -7.069 -4.556 1.00 17.15 ATOM 140 O SER 131 -22.546 -10.501 -5.668 1.00 17.15 ATOM 140 N SER 132 -23.3967 -10.586 -4.209 1.00 15.00 ATOM 141 N SER 132 -23.3967 -10.586 -4.209 1.00 15.00 ATOM 142 H SER 132 -23.3967 -10.586 -4.209 1.00 15.00 ATOM 143 CA SER 132 -24.674 -11.250 -6.218 1.00 21.62 ATOM 144 CB SER 132 -25.266 -12.616 -5.893 1.00 16.00 ATOM 145 OG SER 132 -26.016 -5.893 1.00 16.00 ATOM 146 G SER 132 -26.016 -12.944 -4.179 1.00 15.00 ATOM 147 C SER 132 -26.016 -12.944 -4.179 1.00 15.00 ATOM 148 O SER 132 -26.515 10.544 -7.547 1.00 20.07 ATOM 149 N LYS 133 -25.566 -9.063 -6.118 1.00 21.87 ATOM 150 H LYS 133 -25.606 -9.063 -6.118 1.00 21.87 ATOM 150 C LYS 133 -26.406 -7.916 -6.517 1.00 15.00 ATOM 151 CA LYS 133 -27.684 -8.364 -4.354 1.00 21.07 ATOM 153 CG LYS 133 -27.684 -8.364 -4.355 1.00 23.08 ATOM 153 CG LYS 133 -27.684 -8.364 -4.354 1.00 21.07 ATOM 154 CD LYS 133 -29.9174 -8.110 -4.320 1.00 27.36 ATOM 155 CE LYS 133 -29.9174 -8.110 -4.320 1.00 27.36 ATOM 156 NZ LYS 133 -31.323 -7.515 -5.345 1.00 21.56 ATOM 157 HZ1 LYS 133 -31.362 -7.551 -5.345 1.00 21.56 ATOM 158 HZ2 LYS 133 -31.353 -6.654 -4.760 1.00 15.00 ATOM 159 HZ3 LYS 133 -31.353 -6.654 -4.760 1.00 15.00 ATOM 160 C LYS 133 -25.579 -6.876 -7.194 1.00 15.00 ATOM 161 C LYS 133 -24.378 -6.801 -7.007 1.00 17.94 ATOM 162 N THR 134 -26.260 -6.052 -7.983 1.00 22.97 ATOM 163 H THR 134 -26.540 -5.037 -10.792 1.00 24.32 ATOM 164 CA THR 134 -26.540 -5.037 -10.792 1.00 24.32 ATOM 165 CB THR 134 -26.4987 -3.798 -7.559 1.00 22.97 ATOM 168 CC THR 134 -26.4987 -3.798 -7.559 1.00 22.97 ATOM 169 C THR 134 -26.4987 -3.798 -7.559 1.00 22.97 ATOM 169 C THR 134 -26.4987 -3.798 -7.559 1.00 22.97 ATOM 169 C THR 134 -26.4987 -3.798 -7.559 1.00 24.59 ATOM 169 C THR 134 -26.540 -5.037 -10.792 1.00 24.32 ATOM 169 C THR 134 -26.540 -5.037 -10.792 1.00 24.59 ATOM 177 CGZ THR 135 -22.964 -3.469 -6.386 1.00 35.98 ATOM 178 C THR 134 -26.4987 -3.798 -7.559 1.00 32.51 ATOM 176 C THR 135 -22.966 -4.77 | ATOM | 135 | CA | | | - - · - · - |
| ATOM 138 HG SER 131 -23.329 -7.069 -4.559 1.00 15.00 ATOM 139 C SER 131 -22.546 -10.501 -5.668 1.00 17.15 ATOM 140 O SER 131 -22.546 -10.853 -6.786 1.00 17.15 ATOM 141 N SER 132 -23.756 -10.853 -6.786 1.00 14.30 ATOM 141 N SER 132 -23.756 -10.856 -4.209 1.00 15.00 ATOM 142 H SER 132 -23.967 -10.586 -4.209 1.00 15.00 ATOM 143 CA SER 132 -25.266 -12.616 -5.893 1.00 21.62 ATOM 144 CB SER 132 -25.266 -12.616 -5.893 1.00 21.62 ATOM 145 OG SER 132 -26.203 -12.324 -4.894 1.00 23.84 ATOM 146 HG SER 132 -26.203 -12.324 -4.894 1.00 23.84 ATOM 147 C SER 132 -26.503 -12.544 -4.199 1.00 15.00 ATOM 149 N LYS 133 -25.606 -9.063 -6.118 1.00 20.07 ATOM 149 N LYS 133 -25.606 -9.063 -6.118 1.00 21.87 ATOM 150 H LYS 133 -24.904 -8.969 -5.397 1.00 15.00 ATOM 151 CA LYS 133 -24.904 -8.969 -5.397 1.00 15.00 ATOM 152 CB LYS 133 -27.024 -7.309 -5.256 1.00 23.08 ATOM 153 CG LYS 133 -27.024 -7.309 -5.256 1.00 23.08 ATOM 155 CE LYS 133 -27.024 -7.309 -5.256 1.00 23.08 ATOM 155 CE LYS 133 -27.024 -7.309 -5.256 1.00 23.08 ATOM 155 CE LYS 133 -27.024 -7.309 -5.256 1.00 23.08 ATOM 156 NZ LYS 133 -27.024 -7.309 -5.256 1.00 23.08 ATOM 157 HZ1 LYS 133 -31.323 -7.515 -5.345 1.00 27.36 ATOM 158 HZ2 LYS 133 -31.323 -7.515 -6.218 1.00 27.36 ATOM 159 HZ3 LYS 133 -31.822 -7.515 -6.218 1.00 15.00 ATOM 160 C LYS 133 -31.323 -7.515 -6.218 1.00 15.00 ATOM 160 C LYS 133 -31.323 -7.515 -6.218 1.00 15.00 ATOM 160 C LYS 133 -31.323 -7.515 -6.218 1.00 15.00 ATOM 160 C LYS 133 -31.323 -7.515 -6.206 1.00 23.56 ATOM 161 O LYS 133 -24.904 -8.969 -7.996 1.00 24.32 ATOM 162 N THR 134 -26.260 -6.805 -7.998 1.00 22.95 ATOM 163 H THR 134 -26.260 -6.805 -7.998 1.00 22.57 ATOM 167 HG1 THR 134 -26.260 -6.805 -7.998 1.00 22.95 ATOM 169 C THR 134 -26.260 -6.805 -7.998 1.00 22.95 ATOM 169 C THR 134 -26.260 -6.805 -7.998 1.00 22.95 ATOM 169 C THR 134 -26.260 -6.805 -7.998 1.00 22.95 ATOM 167 HG1 THR 134 -26.260 -6.806 -7.7907 1.00 15.00 ATOM 169 C THR 134 -26.260 -6.806 -7.7909 1.00 24.32 ATOM 167 HG1 THR 134 -26.260 -6.806 -7.7909 1.00 24.59 ATOM 170 O THR 134 -26.260 -6.806 | ATOM | 136 | CB | SER | | |
| ATOM 139 C SER 131 -22.546 -10.501 -5.668 1.00 17.15 ATOM 140 O SER 131 -22.236 -10.853 -6.786 1.00 14.30 ATOM 141 N SER 132 -23.756 -10.731 -5.187 1.00 20.15 ATOM 142 H SER 132 -23.967 -10.586 -4.209 1.00 15.00 ATOM 143 CA SER 132 -24.674 -11.250 -6.218 1.00 21.62 ATOM 144 CB SER 132 -25.266 -12.616 -5.893 1.00 16.00 ATOM 145 OG SER 132 -26.203 -12.324 -4.81 1.00 21.62 ATOM 146 NG SER 132 -26.016 -12.944 -4.179 1.00 15.00 ATOM 147 C SER 132 -25.727 -10.268 -6.671 1.00 20.07 ATOM 148 O SER 132 -25.556 -9.063 -6.118 1.00 21.87 ATOM 149 N LYS 133 -25.606 -9.063 -6.118 1.00 21.87 ATOM 150 H LYS 133 -24.904 -8.969 -5.397 1.00 15.00 ATOM 151 CA LYS 133 -24.904 -8.969 -5.397 1.00 15.00 ATOM 152 CB LYS 133 -27.684 -8.364 -4.354 1.00 23.08 ATOM 153 CG LYS 133 -27.684 -8.364 -4.354 1.00 23.07 ATOM 154 CD LYS 133 -27.684 -8.364 -4.354 1.00 23.07 ATOM 155 CE LYS 133 -29.919 -7.884 -5.670 1.00 30.56 ATOM 156 NZ LYS 133 -31.323 -7.515 -5.345 1.00 27.36 ATOM 157 HZ1 LYS 133 -31.323 -7.515 -5.345 1.00 27.36 ATOM 158 HZ2 LYS 133 -31.323 -7.515 -5.345 1.00 21.56 ATOM 160 C LYS 133 -31.323 -7.515 -5.345 1.00 21.56 ATOM 160 C LYS 133 -31.333 -6.654 -4.760 1.00 30.56 ATOM 161 O LYS 133 -31.323 -7.515 -5.345 1.00 21.56 ATOM 160 C LYS 133 -31.333 -6.654 -7.760 1.00 15.00 ATOM 161 O LYS 133 -24.979 -6.876 -7.194 1.00 22.95 ATOM 160 C LYS 133 -31.333 -6.654 -7.760 1.00 15.00 ATOM 160 C LYS 133 -31.333 -6.654 -7.760 1.00 15.00 ATOM 160 C LYS 133 -24.378 -6.801 -7.007 1.00 17.94 ATOM 160 C LYS 133 -24.378 -6.801 -7.007 1.00 17.94 ATOM 160 C LYS 133 -24.378 -6.801 -7.007 1.00 17.94 ATOM 160 C THR 134 -26.540 -5.037 -10.792 1.00 22.95 ATOM 160 C THR 134 -26.540 -5.037 -10.792 1.00 24.32 ATOM 161 O THR 134 -26.540 -5.037 -10.792 1.00 24.32 ATOM 163 H THR 134 -26.540 -5.037 -10.792 1.00 24.32 ATOM 160 C THR 134 -26.540 -5.037 -10.792 1.00 24.32 ATOM 161 O THR 134 -26.540 -5.037 -10.792 1.00 24.32 ATOM 160 C THR 134 -26.540 -5.037 -10.792 1.00 24.32 ATOM 160 C THR 134 -26.540 -5.037 -10.792 1.00 22.97 ATOM 174 CB THR 135 -22.964 -3.469 -6.38 | MOTA | 137 | OG | SER | | |
| ATOM 140 | ATOM | 138 | HG | | | |
| ATOM 141 N SER 132 -23.756 -10.731 -5.187 1.00 20.15 ATOM 142 H SER 132 -23.967 -10.586 -4.209 1.00 15.00 ATOM 143 CA SER 132 -24.674 -11.250 -6.218 1.00 21.62 ATOM 144 CB SER 132 -25.266 -12.616 -5.893 1.00 16.00 ATOM 145 OG SER 132 -26.203 -12.324 -4.894 1.00 23.84 ATOM 146 NG SER 132 -26.016 -12.944 -4.179 1.00 15.00 ATOM 147 C SER 132 -25.727 -10.268 -6.671 1.00 20.07 ATOM 148 O SER 132 -25.5727 -10.268 -6.671 1.00 20.07 ATOM 149 N LYS 133 -25.606 -9.063 -6.118 1.00 20.27 ATOM 149 N LYS 133 -25.606 -9.063 -6.118 1.00 21.87 ATOM 150 H LYS 133 -27.606 -7.916 -6.517 1.00 19.23 ATOM 151 CA LYS 133 -27.024 -7.309 -5.256 1.00 23.08 ATOM 152 CB LYS 133 -27.684 -8.364 -4.354 1.00 21.07 ATOM 153 CG LYS 133 -27.684 -8.364 -4.354 1.00 21.07 ATOM 154 CD LYS 133 -29.174 -8.110 -4.320 1.00 27.36 ATOM 155 CE LYS 133 -29.174 -8.110 -4.320 1.00 27.36 ATOM 156 NZ LYS 133 -29.999 -7.884 -5.670 1.00 30.56 ATOM 157 HZ1 LYS 133 -31.323 -7.515 -5.345 1.00 21.56 ATOM 158 HZ2 LYS 133 -31.323 -7.515 -5.345 1.00 21.50 ATOM 160 C LYS 133 -31.323 -7.515 -5.345 1.00 21.50 ATOM 160 C LYS 133 -25.579 -6.876 -7.194 1.00 15.00 ATOM 161 O LYS 133 -25.579 -6.876 -7.194 1.00 17.94 ATOM 162 N THR 134 -26.260 -6.052 -7.983 1.00 22.95 ATOM 163 CB THR 134 -26.260 -6.052 -7.983 1.00 22.95 ATOM 165 CB THR 134 -26.260 -6.052 -7.983 1.00 22.95 ATOM 166 OG1 THR 134 -26.260 -6.052 -7.983 1.00 22.95 ATOM 167 HG1 THR 134 -26.260 -6.052 -7.983 1.00 22.95 ATOM 168 CG2 THR 134 -26.232 -4.411 -11.466 1.00 15.00 ATOM 169 C THR 134 -26.232 -4.411 -11.466 1.00 15.00 ATOM 167 HG1 THR 134 -26.232 -4.411 -11.466 1.00 15.00 ATOM 167 HG1 THR 135 -23.717 -3.352 -7.690 1.00 38.43 ATOM 168 CG2 THR 134 -26.260 -6.052 -7.983 1.00 22.95 ATOM 167 HG1 THR 135 -22.964 -3.469 -6.386 1.00 36.01 ATOM 171 N THR 135 -22.964 -3.469 -6.386 1.00 36.01 ATOM 172 H THR 135 -22.966 -4.471 -11.466 1.00 36.01 ATOM 175 HG1 THR 135 -22.2964 -3.469 -6.386 1.00 35.55 ATOM 176 HG1 THR 135 -22.2964 -3.469 -6.386 1.00 35.55 ATOM 176 HG1 THR 135 -22.2964 -3.469 -6.534 1.00 30.60 ATOM 177 CG2 THR 1 | ATOM | 139 | C | SER | | |
| ATOM 141 N SER 132 -23.756 -10.731 -5.187 1.00 20.15 ATOM 142 H SER 132 -24.674 -11.250 -6.218 1.00 21.62 ATOM 143 CA SER 132 -24.674 -11.250 -6.218 1.00 21.62 ATOM 144 CB SER 132 -25.266 -12.616 -5.893 1.00 16.00 ATOM 145 OG SER 132 -26.203 -12.324 -4.894 1.00 23.84 ATOM 146 HG SER 132 -26.203 -12.324 -4.894 1.00 23.84 ATOM 147 C SER 132 -26.203 -12.324 -4.894 1.00 23.84 ATOM 148 O SER 132 -25.727 -10.268 -6.671 1.00 20.07 ATOM 149 N LYS 133 -25.606 -9.063 -6.118 1.00 21.87 ATOM 150 H LYS 133 -25.606 -9.063 -6.118 1.00 21.87 ATOM 151 CA LYS 133 -24.904 -8.969 -5.397 1.00 15.00 ATOM 152 CB LYS 133 -27.624 -7.309 -5.256 1.00 23.08 ATOM 153 CG LYS 133 -27.624 -8.364 -4.354 1.00 21.07 ATOM 154 CD LYS 133 -27.684 -8.364 -4.354 1.00 21.07 ATOM 155 CE LYS 133 -29.174 -8.110 -4.320 1.00 27.36 ATOM 156 NZ LYS 133 -31.323 -7.515 -5.345 1.00 21.56 ATOM 157 HZ1 LYS 133 -31.323 -7.515 -5.345 1.00 21.56 ATOM 158 HZ2 LYS 133 -31.323 -7.515 -5.345 1.00 15.00 ATOM 159 HZ3 LYS 133 -31.323 -7.515 -6.218 1.00 15.00 ATOM 160 C LYS 133 -25.579 -6.876 -7.194 1.00 20.10 ATOM 161 O LYS 133 -24.378 -6.801 -7.007 1.00 17.94 ATOM 162 N THR 134 -26.260 -6.052 -7.983 1.00 22.95 ATOM 163 CB THR 134 -26.232 -4.411 -11.456 1.00 15.00 ATOM 164 CA THR 134 -26.232 -4.411 -11.456 1.00 15.00 ATOM 165 CB THR 134 -26.568 -3.461 -6.603 1.00 38.43 ATOM 167 HG1 THR 134 -26.523 -4.411 -11.456 1.00 15.00 ATOM 167 HG1 THR 134 -26.523 -4.411 -11.456 1.00 15.00 ATOM 167 HG1 THR 134 -26.523 -4.411 -11.456 1.00 15.00 ATOM 167 HG1 THR 134 -26.523 -4.411 -11.456 1.00 15.00 ATOM 167 HG1 THR 134 -26.527 -4.411 -11.456 1.00 15.00 ATOM 167 HG1 THR 134 -26.529 -3.461 -6.603 1.00 38.43 ATOM 167 HG1 THR 135 -23.717 -3.352 -7.698 1.00 32.51 ATOM 167 HG1 THR 134 -26.529 -4.411 -11.456 1.00 15.00 ATOM 171 N THR 134 -26.529 -4.411 -11.456 1.00 15.00 ATOM 172 H THR 135 -23.717 -3.352 -7.698 1.00 32.51 ATOM 173 CA THR 135 -22.866 -4.766 -5.341 1.00 36.01 ATOM 175 HG1 THR 135 -22.866 -4.766 -5.404 1.00 36.01 ATOM 175 HG1 THR 135 -22.866 -5.404 1.00 36.02 ATOM 175 HG1 THR 135 | ATOM | 140 | 0 | SER | 131 | |
| ATOM 142 H SER 132 -23.967 -10.586 -4.209 1.00 21.62 ATOM 143 CA SER 132 -24.674 -11.250 -6.218 1.00 21.62 ATOM 145 OG SER 132 -25.266 -12.616 -5.893 1.00 16.00 ATOM 145 OG SER 132 -26.203 -12.324 -4.894 1.00 23.84 ATOM 146 HG SER 132 -26.016 -12.944 -4.179 1.00 15.00 ATOM 147 C SER 132 -26.5016 -12.944 -4.179 1.00 15.00 ATOM 147 C SER 132 -26.535 -10.544 -7.547 1.00 20.07 ATOM 148 O SER 132 -26.535 -10.544 -7.547 1.00 20.07 ATOM 148 O SER 132 -26.535 -10.544 -7.547 1.00 20.27 ATOM 148 O SER 132 -26.606 -9.063 -6.118 1.00 21.87 ATOM 150 H LYS 133 -24.904 -8.969 -5.397 1.00 15.00 ATOM 151 CA LYS 133 -24.904 -8.969 -5.397 1.00 15.00 ATOM 152 CB LYS 133 -27.024 -7.309 -5.256 1.00 23.08 ATOM 153 CG LYS 133 -27.024 -7.309 -5.256 1.00 23.08 ATOM 155 CB LYS 133 -27.684 -8.364 -4.354 1.00 21.07 ATOM 155 CE LYS 133 -29.919 -7.884 -5.670 1.00 27.36 ATOM 155 CE LYS 133 -29.919 -7.884 -5.670 1.00 27.36 ATOM 155 CE LYS 133 -29.919 -7.884 -5.670 1.00 27.36 ATOM 156 NZ LYS 133 -31.323 -7.515 -5.345 1.00 21.56 ATOM 157 HZ1 LYS 133 -31.323 -7.515 -5.345 1.00 21.56 ATOM 159 HZ3 LYS 133 -31.333 -6.654 -4.760 1.00 15.00 ATOM 159 HZ3 LYS 133 -31.333 -6.654 -4.760 1.00 15.00 ATOM 160 C LYS 133 -24.378 -6.801 -7.007 1.00 17.94 ATOM 161 O LYS 133 -24.378 -6.801 -7.007 1.00 17.94 ATOM 163 H THR 134 -26.540 -5.037 -10.792 1.00 24.59 ATOM 166 CB THR 134 -26.540 -5.037 -10.792 1.00 24.32 ATOM 166 CG THR 134 -26.540 -5.037 -10.792 1.00 24.32 ATOM 167 HG1 THR 134 -26.540 -5.037 -10.792 1.00 24.32 ATOM 168 CG2 THR 134 -26.540 -5.037 -10.799 1.00 24.32 ATOM 169 C THR 134 -26.540 -5.037 -10.799 1.00 24.59 ATOM 169 C THR 134 -26.540 -5.386 1.00 15.00 ATOM 171 N THR 135 -22.2964 -3.461 -6.603 1.00 36.01 ATOM 172 H THR 135 -22.2964 -3.461 -6.603 1.00 36.01 ATOM 173 CA THR 135 -22.2964 -3.461 -6.603 1.00 36.01 ATOM 174 CB THR 135 -22.2964 -3.460 -6.386 1.00 35.98 ATOM 175 CGI THR 135 -22.2964 -3.460 -6.386 1.00 36.01 ATOM 175 CGI THR 135 -22.2964 -3.460 -6.386 1.00 30.55 ATOM 177 CGI THR 135 -22.255 -6.094 -7.312 1.00 35.55 ATOM 175 CGI THR 135 -2 | 4 | 141 | N | SER | 132 | |
| ATOM 143 CA SER 132 -24.674 -11.250 -6.218 1.00 21.62 ATOM 144 CB SER 132 -25.266 -12.324 -4.894 1.00 23.84 ATOM 146 HG SER 132 -26.203 -12.324 -4.894 1.00 23.84 ATOM 146 HG SER 132 -26.016 -12.944 -4.179 1.00 15.00 ATOM 147 C SER 132 -26.5727 -10.268 -6.671 1.00 20.07 ATOM 148 O SER 132 -26.535 -10.544 -7.547 1.00 20.27 ATOM 149 N LYS 133 -25.606 -9.063 -6.118 1.00 21.87 ATOM 150 H LYS 133 -24.904 -8.969 -5.397 1.00 15.00 ATOM 151 CA LYS 133 -24.904 -8.969 -5.397 1.00 15.00 ATOM 152 CB LYS 133 -27.024 -7.309 -5.256 1.00 23.08 ATOM 153 CG LYS 133 -27.684 -8.364 -4.354 1.00 21.07 ATOM 154 CD LYS 133 -27.684 -8.364 -4.354 1.00 21.07 ATOM 155 CE LYS 133 -29.174 -8.110 -4.320 1.00 27.36 ATOM 156 NZ LYS 133 -31.323 -7.515 -5.345 1.00 21.56 ATOM 157 HZ1 LYS 133 -31.862 -7.351 -6.218 1.00 21.56 ATOM 158 HZ2 LYS 133 -31.862 -7.351 -6.218 1.00 15.00 ATOM 159 HZ3 LYS 133 -31.862 -7.351 -6.218 1.00 15.00 ATOM 160 C LYS 133 -27.559 -6.876 -7.194 1.00 20.10 ATOM 161 O LYS 133 -24.378 -6.801 -7.007 1.00 17.94 ATOM 162 N THR 134 -26.260 -6.052 -7.983 1.00 22.95 ATOM 163 H THR 134 -26.260 -8.052 -7.983 1.00 22.95 ATOM 165 CB THR 134 -26.260 -8.056 1.00 27.89 ATOM 166 CA THR 134 -26.260 -6.052 -7.983 1.00 22.95 ATOM 167 HG1 THR 134 -26.232 -4.411 -11.456 1.00 15.00 ATOM 169 C THR 134 -26.249 -4.274 -9.592 1.00 24.59 ATOM 169 C THR 134 -26.232 -4.411 -11.456 1.00 15.00 ATOM 169 C THR 134 -26.249 -7.559 1.00 22.97 ATOM 169 C THR 134 -26.249 -7.559 1.00 22.97 ATOM 169 C THR 134 -26.232 -4.411 -11.456 1.00 15.00 ATOM 170 N THR 134 -26.232 -4.411 -11.456 1.00 15.00 ATOM 171 N THR 134 -26.249 -3.555 -6.585 1.00 32.51 ATOM 172 H THR 135 -22.964 -3.469 -6.386 1.00 30.60 ATOM 173 CA THR 135 -22.964 -3.469 -6.386 1.00 35.55 ATOM 175 NGT THR 135 -22.255 -6.094 -7.312 1.00 15.00 ATOM 176 HG1 THR 135 -22.266 -5.388 -7.488 1.00 30.60 ATOM 177 CG2 THR 135 -22.866 -4.776 -5.264 1.00 35.55 ATOM 176 NGT THR 135 -22.266 -5.386 -7.381 1.00 30.25 | | 142 | H | SER | 132 | |
| ATOM 144 CB SER 132 -25.266 -12.616 -5.893 1.00 23.84 ATOM 145 OG SER 132 -26.203 -12.324 -4.894 1.00 23.84 ATOM 146 HG SER 132 -26.016 -12.944 -4.179 1.00 15.00 ATOM 147 C SER 132 -25.727 -10.268 -6.671 1.00 20.07 ATOM 148 O SER 132 -25.525 -10.544 -7.547 1.00 20.27 ATOM 149 N LYS 133 -25.606 -9.063 -6.118 1.00 21.87 ATOM 150 H LYS 133 -24.904 -8.969 -5.397 1.00 15.00 ATOM 151 CA LYS 133 -24.904 -8.969 -5.397 1.00 15.00 ATOM 152 CB LYS 133 -27.024 -7.309 -5.256 1.00 23.08 ATOM 153 CG LYS 133 -27.684 -8.364 -4.354 1.00 21.07 ATOM 154 CD LYS 133 -27.684 -8.364 -4.354 1.00 21.07 ATOM 155 CE LYS 133 -29.939 -7.884 -5.670 1.00 30.56 ATOM 156 NZ LYS 133 -31.323 -7.515 -5.345 1.00 21.56 ATOM 157 HZ1 LYS 133 -31.323 -7.515 -5.345 1.00 21.56 ATOM 158 HZ2 LYS 133 -31.323 -7.515 -5.345 1.00 15.00 ATOM 160 C LYS 133 -25.579 -6.876 -7.194 1.00 15.00 ATOM 161 O LYS 133 -25.579 -6.876 -7.194 1.00 20.10 ATOM 162 N THR 134 -26.260 -6.052 -7.983 1.00 22.95 ATOM 163 CB THR 134 -26.260 -6.052 -7.983 1.00 22.95 ATOM 166 CG THR 134 -26.540 -5.037 -10.792 1.00 24.32 ATOM 167 HGI THR 134 -26.540 -5.037 -10.792 1.00 24.32 ATOM 169 C THR 134 -26.540 -5.037 -10.792 1.00 24.59 ATOM 169 C THR 134 -26.540 -7.037 -9.968 1.00 22.95 ATOM 169 C THR 134 -26.540 -7.037 -9.968 1.00 22.95 ATOM 169 C THR 134 -26.540 -7.037 -9.968 1.00 22.97 ATOM 169 C THR 134 -26.540 -7.037 -9.968 1.00 22.97 ATOM 167 HGI THR 134 -26.556 -3.461 -6.603 1.00 35.50 ATOM 169 C THR 134 -26.540 -7.037 -9.968 1.00 22.97 ATOM 169 C THR 134 -26.644 -2.897 -9.968 1.00 22.97 ATOM 169 C THR 134 -26.568 -3.461 -6.603 1.00 35.50 ATOM 170 O THR 134 -26.569 -3.369 -6.386 1.00 35.00 ATOM 171 N THR 135 -22.964 -3.469 -6.386 1.00 36.01 ATOM 172 H THR 135 -22.964 -3.469 -6.386 1.00 36.01 ATOM 173 CG THR 135 -22.964 -3.469 -6.386 1.00 35.55 ATOM 174 CB THR 135 -22.966 -4.776 -5.264 1.00 35.55 ATOM 175 CGI THR 135 -22.866 -4.776 -5.264 1.00 35.55 ATOM 177 CG2 THR 135 -22.866 -5.404 -7.502 1.00 35.55 | | 143 | CA | SER | 132 | |
| ATOM 145 OG SER 132 -26.203 -12.324 -4.894 1.00 23.84 ATOM 146 HG SER 132 -26.016 -12.944 -4.179 1.00 15.00 ATOM 147 C SER 132 -26.535 -10.544 -7.547 1.00 20.07 ATOM 148 O SER 132 -26.535 -10.544 -7.547 1.00 20.27 ATOM 149 N LYS 133 -25.606 -9.063 -6.671 1.00 20.27 ATOM 149 N LYS 133 -24.904 -8.969 -5.397 1.00 15.00 ATOM 150 H LYS 133 -24.904 -8.969 -5.397 1.00 15.00 ATOM 151 CA LYS 133 -26.406 -7.916 -6.517 1.00 19.23 ATOM 152 CB LYS 133 -27.684 -8.364 -4.354 1.00 21.07 ATOM 153 CG LYS 133 -27.684 -8.364 -4.354 1.00 21.07 ATOM 154 CD LYS 133 -29.174 -8.110 -4.320 1.00 27.36 ATOM 155 CE LYS 133 -29.174 -8.110 -4.320 1.00 27.36 ATOM 156 NZ LYS 133 -31.323 -7.515 -5.345 1.00 21.56 ATOM 157 HZ1 LYS 133 -31.323 -7.515 -5.345 1.00 21.56 ATOM 159 HZ3 LYS 133 -31.323 -7.515 -6.218 1.00 15.00 ATOM 159 HZ3 LYS 133 -31.753 -8.299 -4.811 1.00 15.00 ATOM 160 C LYS 133 -25.579 -6.876 -7.194 1.00 15.00 ATOM 161 O LYS 133 -24.378 -6.801 -7.007 1.00 17.94 ATOM 162 N THR 134 -26.260 -6.052 -7.983 1.00 22.95 ATOM 163 H THR 134 -26.260 -6.052 -7.983 1.00 22.95 ATOM 164 CA THR 134 -26.260 -6.052 -7.983 1.00 22.95 ATOM 165 CB THR 134 -26.260 -4.274 -9.592 1.00 24.59 ATOM 167 HG1 THR 134 -26.260 -4.274 -9.592 1.00 24.59 ATOM 167 HG1 THR 134 -26.260 -4.274 -9.592 1.00 24.59 ATOM 167 HG1 THR 134 -26.260 -4.274 -9.592 1.00 24.32 ATOM 167 HG1 THR 134 -26.260 -4.274 -9.592 1.00 24.32 ATOM 167 HG1 THR 134 -26.260 -4.274 -9.592 1.00 24.32 ATOM 167 HG1 THR 134 -26.260 -4.274 -9.592 1.00 24.32 ATOM 167 HG1 THR 134 -26.260 -4.274 -9.592 1.00 24.32 ATOM 167 HG1 THR 134 -26.260 -4.274 -9.592 1.00 24.59 ATOM 167 HG1 THR 134 -26.260 -6.052 -7.983 1.00 22.97 ATOM 167 HG1 THR 134 -26.260 -6.060 -7.079 1.00 15.00 ATOM 168 CG2 THR 134 -26.260 -6.060 -7.079 1.00 15.00 ATOM 168 CG2 THR 134 -26.260 -6.060 -7.079 1.00 24.32 ATOM 167 HG1 THR 134 -26.260 -6.060 -7.079 1.00 24.32 ATOM 167 HG1 THR 134 -26.260 -6.060 -7.079 1.00 24.32 ATOM 167 HG1 THR 134 -26.260 -7.079 1.00 24.32 ATOM 167 HG1 THR 135 -22.266 -4.276 -6.386 1.00 36.01 ATOM 175 CG2 THR 135 -22. | | | CB | SER | 132 | |
| ATOM 146 HG SER 132 -26.016 -12.944 -4.179 | | | OG | SER | 132 | |
| ATOM 148 O SER 132 | | | HG | | 132 | |
| ATOM 148 O SER 132 -26.555 -10.544 -7.547 1.00 20.27 ATOM 149 N LYS 133 -25.606 -9.063 -6.118 1.00 21.87 ATOM 150 H LYS 133 -24.904 -8.969 -5.397 1.00 15.00 ATOM 151 CA LYS 133 -24.904 -7.309 -5.256 1.00 23.08 ATOM 152 CB LYS 133 -27.024 -7.309 -5.256 1.00 23.08 ATOM 153 CG LYS 133 -27.684 -8.364 -4.354 1.00 21.07 ATOM 154 CD LYS 133 -29.174 -8.110 -4.320 1.00 27.36 ATOM 155 CE LYS 133 -29.174 -8.110 -4.320 1.00 27.36 ATOM 155 NZ LYS 133 -29.174 -8.110 -4.320 1.00 27.36 ATOM 156 NZ LYS 133 -31.323 -7.515 -5.345 1.00 21.56 ATOM 157 HZ1 LYS 133 -31.862 -7.351 -6.218 1.00 15.00 ATOM 158 HZ2 LYS 133 -31.323 -7.515 -5.345 1.00 21.56 ATOM 158 HZ2 LYS 133 -31.333 -6.654 -4.760 1.00 15.00 ATOM 160 C LYS 133 -25.579 -6.876 -7.194 1.00 20.10 ATOM 161 O LYS 133 -25.579 -6.876 -7.194 1.00 22.95 ATOM 162 N THR 134 -26.260 -6.052 -7.983 1.00 22.95 ATOM 163 H THR 134 -26.260 -6.052 -7.983 1.00 22.95 ATOM 164 CA THR 134 -25.556 -4.879 -8.561 1.00 27.89 ATOM 165 CB THR 134 -26.240 -5.037 -10.792 1.00 24.59 ATOM 166 OG1 THR 134 -26.232 -4.411 -11.456 1.00 15.00 ATOM 167 HG1 THR 134 -26.232 -4.411 -11.456 1.00 15.00 ATOM 168 CG2 THR 134 -26.232 -4.411 -11.456 1.00 15.00 ATOM 169 C THR 134 -26.232 -4.411 -11.456 1.00 15.00 ATOM 169 C THR 134 -26.232 -4.411 -11.456 1.00 15.00 ATOM 169 C THR 134 -26.232 -4.411 -11.456 1.00 22.97 ATOM 169 C THR 134 -26.232 -4.411 -11.456 1.00 35.98 ATOM 170 O THR 134 -26.232 -4.411 -11.456 1.00 35.98 ATOM 171 N THR 135 -23.717 -3.352 -7.690 1.00 38.43 ATOM 172 H THR 135 -22.964 -3.469 -6.386 1.00 35.98 ATOM 173 CA THR 135 -22.964 -3.469 -6.386 1.00 36.00 ATOM 174 CB THR 135 -22.964 -3.469 -6.386 1.00 35.55 ATOM 175 OG1 THR 135 -22.965 -4.976 -5.264 1.00 35.55 ATOM 176 GG1 THR 135 -22.964 -7.476 -5.266 1.00 35.55 ATOM 177 CG2 THR 135 -22.966 -4.776 -5.266 1.00 35.55 ATOM 177 CG2 THR 135 -22.949 -2.266 -5.404 1.00 35.55 | | | | SER | 132 | |
| ATOM 149 N LYS 133 -24.904 -8.969 -5.397 1.00 15.00 ATOM 151 CA LYS 133 -24.904 -8.969 -5.397 1.00 15.00 ATOM 151 CA LYS 133 -26.406 -7.916 -6.517 1.00 19.23 ATOM 152 CB LYS 133 -27.024 -7.309 -5.256 1.00 23.08 ATOM 153 CG LYS 133 -27.684 -8.364 -4.354 1.00 21.07 ATOM 155 CE LYS 133 -29.174 -8.110 -4.320 1.00 27.36 ATOM 155 CE LYS 133 -29.939 -7.884 -5.670 1.00 30.56 ATOM 155 CE LYS 133 -31.323 -7.515 -5.345 -1.00 21.56 ATOM 157 HZ1 LYS 133 -31.862 -7.351 -6.218 1.00 15.00 ATOM 158 HZ2 LYS 133 -31.323 -7.515 -6.218 1.00 15.00 ATOM 159 HZ3 LYS 133 -31.753 -8.299 -4.811 1.00 15.00 ATOM 160 C LYS 133 -25.579 -6.876 -7.194 1.00 20.10 ATOM 161 O LYS 133 -25.579 -6.876 -7.194 1.00 20.10 ATOM 162 N THR 134 -26.260 -6.052 -7.983 1.00 22.95 ATOM 163 H THR 134 -27.275 -6.130 -8.036 1.00 15.00 ATOM 164 CA THR 134 -25.556 -4.879 -8.561 1.00 27.89 ATOM 165 CB THR 134 -26.540 -5.037 -10.792 1.00 24.59 ATOM 166 CG2 THR 134 -26.540 -5.037 -10.792 1.00 24.59 ATOM 169 C THR 134 -26.540 -5.037 -10.792 1.00 24.59 ATOM 169 CG2 THR 134 -26.540 -5.037 -10.792 1.00 24.59 ATOM 169 CG2 THR 134 -26.540 -5.037 -10.792 1.00 24.59 ATOM 169 CG2 THR 134 -26.540 -5.037 -10.792 1.00 24.59 ATOM 169 CG2 THR 134 -26.540 -5.037 -10.792 1.00 24.59 ATOM 169 CG2 THR 134 -26.540 -5.037 -10.792 1.00 24.59 ATOM 169 CG2 THR 134 -26.540 -5.037 -10.792 1.00 24.59 ATOM 169 CG2 THR 134 -26.540 -5.037 -10.792 1.00 24.59 ATOM 169 CG2 THR 134 -26.540 -5.037 -10.792 1.00 24.59 ATOM 169 CG2 THR 134 -26.540 -5.037 -10.792 1.00 24.59 ATOM 169 CG2 THR 134 -26.645 -5.386 -7.488 1.00 36.01 ATOM 170 O THR 134 -22.987 -3.798 -7.559 1.00 32.51 ATOM 170 O THR 134 -22.987 -3.798 -7.559 1.00 32.51 ATOM 170 O THR 134 -22.986 -3.469 -6.386 1.00 36.02 ATOM 171 N THR 135 -23.292 -3.555 -8.585 1.00 15.00 ATOM 173 CA THR 135 -22.964 -3.469 -6.386 1.00 36.01 ATOM 175 CG2 THR 135 -22.964 -3.469 -6.386 1.00 35.55 ATOM 175 CG2 THR 135 -22.964 -3.469 -6.554 1.00 35.55 ATOM 175 CG2 THR 135 -22.964 -4.776 -5.264 1.00 35.55 ATOM 175 CG2 THR 135 -22.966 -4.776 -5.264 1.00 35.55 ATOM 175 CG | | | | | 132 | |
| ATOM 150 H LYS 133 -24.904 -8.969 -5.397 1.00 15.00 ATOM 151 CA LYS 133 -26.406 -7.916 -6.517 1.00 19.23 ATOM 152 CB LYS 133 -27.024 -7.309 -5.256 1.00 23.08 ATOM 153 CG LYS 133 -27.684 -8.364 -4.354 1.00 21.07 ATOM 153 CG LYS 133 -29.174 -8.110 -4.320 1.00 27.36 ATOM 155 CE LYS 133 -29.939 -7.884 -5.670 1.00 30.56 ATOM 156 NZ LYS 133 -29.939 -7.884 -5.670 1.00 30.56 ATOM 156 NZ LYS 133 -31.323 -7.515 -5.345 1.00 21.56 ATOM 157 HZ1 LYS 133 -31.862 -7.351 -6.218 1.00 15.00 ATOM 158 HZ2 LYS 133 -31.753 -8.299 -4.811 1.00 15.00 ATOM 159 HZ3 LYS 133 -31.333 -6.654 -4.760 1.00 15.00 ATOM 160 C LYS 133 -25.579 -6.876 -7.194 1.00 20.10 ATOM 161 O LYS 133 -25.579 -6.876 -7.194 1.00 20.10 ATOM 162 N THR 134 -26.260 -6.052 -7.983 1.00 22.95 ATOM 163 H THR 134 -26.260 -6.052 -7.983 1.00 22.95 ATOM 165 CB THR 134 -26.498 -4.274 -9.9592 1.00 24.59 ATOM 166 OG1 THR 134 -26.498 -4.274 -9.9592 1.00 24.59 ATOM 166 OG1 THR 134 -26.540 -5.037 -10.792 1.00 24.32 ATOM 167 HG1 THR 134 -26.540 -5.037 -10.792 1.00 24.32 ATOM 169 C THR 134 -26.540 -5.037 -7.559 1.00 32.51 ATOM 169 C THR 134 -26.540 -5.037 -7.590 1.00 32.51 ATOM 169 C THR 134 -26.540 -5.037 -7.690 1.00 32.51 ATOM 170 N THR 135 -23.292 -3.555 -8.585 1.00 15.00 ATOM 172 H THR 135 -23.292 -3.555 -6.386 -7.381 1.00 36.01 ATOM 173 N THR 135 -22.964 -3.469 -6.534 1.00 36.01 ATOM 175 OG1 THR 135 -22.265 -6.094 -7.312 1.00 35.55 ATOM 175 OG1 THR 135 -22.265 -6.094 -7.312 1.00 35.55 ATOM 175 OG1 THR 135 -22.265 -6.094 -7.312 1.00 35.55 ATOM 175 OG1 THR 135 -22.265 -6.094 -7.312 1.00 35.55 ATOM 175 OG1 THR 135 -22.265 -6.094 -7.312 1.00 35.55 ATOM 175 OG2 THR 135 -22.266 -5.404 1.00 35.55 ATOM 175 OG1 THR 135 -22.255 -6.094 -7.312 1.00 35.55 ATOM 175 OG2 THR 135 -22.266 -5.404 1.00 35.55 ATOM 175 OG2 THR 135 -22.266 -5.404 1.00 35.55 ATOM 175 OG2 THR 135 -22.266 -5.404 1.00 35.55 ATOM 175 OG2 THR 135 -22.266 -5.404 1.00 35.55 ATOM 175 OG2 THR 135 -22.266 -5.404 1.00 35.55 ATOM 175 OG2 THR 135 -22.266 -5.404 1.00 35.55 ATOM 175 OG3 THR 135 -22.266 -5.404 1.00 35.55 ATOM 175 OG3 TH | | | | | | -25.606 -9.063 -6.118 1.00 21.87 |
| ATOM 151 CA LYS 133 -26.406 -7.916 -6.517 1.00 19.23 ATOM 152 CB LYS 133 -27.024 -7.309 -5.256 1.00 23.08 ATOM 153 CG LYS 133 -27.024 -8.110 -4.354 1.00 21.07 ATOM 154 CD LYS 133 -29.174 -8.110 -4.320 1.00 27.36 ATOM 155 CE LYS 133 -29.939 -7.884 -5.670 1.00 30.56 ATOM 156 NZ LYS 133 -31.323 -7.515 -5.345 1.00 21.56 ATOM 157 HZ1 LYS 133 -31.323 -7.515 -5.345 1.00 21.56 ATOM 158 HZ2 LYS 133 -31.323 -7.515 -6.218 1.00 15.00 ATOM 159 HZ3 LYS 133 -31.333 -6.654 -4.760 1.00 15.00 ATOM 160 C LYS 133 -25.579 -6.876 -7.194 1.00 20.10 ATOM 161 O LYS 133 -24.378 -6.801 -7.007 1.00 17.94 ATOM 162 N THR 134 -26.260 -6.052 -7.983 1.00 22.95 ATOM 163 H THR 134 -27.275 -6.130 -8.036 1.00 22.95 ATOM 165 CB THR 134 -26.540 -5.037 -10.792 1.00 24.59 ATOM 166 OG1 THR 134 -26.540 -5.037 -10.792 1.00 24.59 ATOM 168 CG2 THR 134 -26.540 -5.037 -10.792 1.00 24.32 ATOM 169 C THR 134 -26.540 -5.037 -9.968 1.00 22.97 ATOM 169 C THR 134 -26.540 -5.037 -7.599 1.00 32.51 ATOM 169 C THR 134 -26.540 -5.037 -10.792 1.00 24.32 ATOM 169 C THR 134 -26.540 -5.037 -10.792 1.00 24.32 ATOM 169 C THR 134 -26.540 -5.037 -10.792 1.00 24.32 ATOM 169 C THR 134 -26.540 -5.037 -10.792 1.00 24.59 ATOM 169 C THR 134 -26.540 -5.037 -10.792 1.00 24.59 ATOM 169 C THR 134 -26.540 -5.037 -10.792 1.00 24.59 ATOM 169 C THR 134 -26.540 -5.037 -10.792 1.00 24.59 ATOM 169 C THR 134 -26.540 -5.037 -10.792 1.00 24.59 ATOM 170 O THR 134 -26.540 -5.037 -10.792 1.00 24.59 ATOM 170 O THR 134 -26.540 -6.503 -7.559 1.00 15.00 ATOM 171 N THR 135 -23.717 -3.352 -7.690 1.00 35.98 ATOM 172 H THR 135 -22.964 -3.469 -6.386 1.00 36.02 ATOM 173 CB THR 135 -22.964 -3.469 -6.386 1.00 36.02 ATOM 174 CB THR 135 -22.964 -3.469 -6.386 1.00 36.02 | | | | | | |
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| ATOM 154 CD LYS 133 -29.174 -8.110 -4.320 1.00 27.36 ATOM 155 CE LYS 133 -29.939 -7.884 -5.670 1.00 30.56 ATOM 156 NZ LYS 133 -31.323 -7.515 -5.345 1.00 21.56 ATOM 157 HZ1 LYS 133 -31.862 -7.351 -6.218 1.00 15.00 ATOM 159 HZ3 LYS 133 -31.753 -8.299 -4.811 1.00 15.00 ATOM 159 HZ3 LYS 133 -31.333 -6.654 -4.760 1.00 15.00 ATOM 160 C LYS 133 -25.579 -6.876 -7.194 1.00 20.10 ATOM 161 O LYS 133 -24.378 -6.801 -7.007 1.00 17.94 ATOM 162 N THR 134 -26.260 -6.052 -7.983 1.00 22.95 ATOM 163 H THR 134 -27.275 -6.130 -8.036 1.00 15.00 ATOM 164 CA THR 134 -25.556 -4.879 -8.561 1.00 27.89 ATOM 165 CB THR 134 -26.498 -4.274 -9.592 1.00 24.59 ATOM 166 OG1 THR 134 -26.540 -5.037 -10.792 1.00 24.59 ATOM 167 HG1 THR 134 -26.540 -5.037 -10.792 1.00 24.32 ATOM 168 CG2 THR 134 -26.044 -2.897 -9.968 1.00 22.97 ATOM 169 C THR 134 -26.044 -2.897 -9.968 1.00 22.97 ATOM 170 O THR 134 -26.044 -2.897 -9.968 1.00 22.97 ATOM 171 N THR 135 -23.717 -3.352 -7.690 1.00 38.43 ATOM 172 H THR 135 -23.717 -3.352 -7.690 1.00 36.02 ATOM 173 CA THR 135 -22.964 -3.469 -6.386 1.00 36.01 ATOM 175 OG1 THR 135 -22.964 -3.469 -6.386 1.00 36.01 ATOM 176 HG1 THR 135 -22.964 -7.312 1.00 25.55 ATOM 177 CG2 THR 135 -22.964 -7.312 1.00 35.55 ATOM 177 CG2 THR 135 -22.964 -7.76 -5.264 1.00 35.55 ATOM 177 CG2 THR 135 -22.966 -4.776 -5.264 1.00 35.55 | | | | | | |
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| ATOM 156 NZ LYS 133 -31.323 -7.515 -5.345 1.00 21.56 ATOM 157 HZ1 LYS 133 -31.862 -7.351 -6.218 1.00 15.00 ATOM 158 HZ2 LYS 133 -31.753 -8.299 -4.811 1.00 15.00 ATOM 159 HZ3 LYS 133 -31.333 -6.654 -4.760 1.00 15.00 ATOM 160 C LYS 133 -25.579 -6.876 -7.194 1.00 20.10 ATOM 161 O LYS 133 -24.378 -6.801 -7.007 1.00 17.94 ATOM 162 N THR 134 -26.260 -6.052 -7.983 1.00 22.95 ATOM 163 H THR 134 -26.260 -6.052 -7.983 1.00 22.95 ATOM 164 CA THR 134 -25.556 -4.879 -8.561 1.00 27.89 ATOM 165 CB THR 134 -26.498 -4.274 -9.592 1.00 24.59 ATOM 166 OGI THR 134 -26.540 -5.037 -10.792 1.00 24.32 ATOM 167 HGI THR 134 -26.540 -5.037 -10.792 1.00 24.32 ATOM 168 CG2 THR 134 -26.044 -2.897 -9.968 1.00 22.97 ATOM 169 C THR 134 -26.044 -2.897 -9.968 1.00 22.97 ATOM 169 C THR 134 -25.556 -3.461 -6.603 1.00 38.43 ATOM 170 O THR 135 -23.717 -3.352 -7.690 1.00 32.51 ATOM 171 N THR 135 -23.717 -3.352 -7.690 1.00 35.98 ATOM 172 H THR 135 -23.717 -3.352 -7.690 1.00 35.98 ATOM 173 CA THR 135 -22.964 -3.469 -6.386 1.00 36.01 ATOM 174 CB THR 135 -22.964 -3.469 -6.534 1.00 36.01 ATOM 175 GGI THR 135 -22.964 -3.469 -6.534 1.00 36.01 ATOM 176 HGI THR 135 -22.255 -6.094 -7.312 1.00 15.00 ATOM 177 CG2 THR 135 -22.266 -5.404 1.00 30.25 ATOM 177 CG2 THR 135 -22.255 -6.094 -7.312 1.00 30.25 | | | | | | -29.939 -7.884 -5.670 1.00 30.56 |
| ATOM 157 HZ1 LYS 133 -31.862 -7.351 -6.218 1.00 15.00 ATOM 158 HZ2 LYS 133 -31.753 -8.299 -4.811 1.00 15.00 ATOM 159 HZ3 LYS 133 -31.333 -6.654 -4.760 1.00 15.00 ATOM 160 C LYS 133 -25.579 -6.876 -7.194 1.00 20.10 ATOM 161 O LYS 133 -24.378 -6.801 -7.007 1.00 17.94 ATOM 162 N THR 134 -26.260 -6.052 -7.983 1.00 22.95 ATOM 163 H THR 134 -26.260 -6.052 -7.983 1.00 22.95 ATOM 164 CA THR 134 -25.556 -4.879 -8.561 1.00 15.00 ATOM 165 CB THR 134 -26.498 -4.274 -9.592 1.00 24.59 ATOM 166 OG1 THR 134 -26.540 -5.037 -10.792 1.00 24.32 ATOM 167 HG1 THR 134 -26.232 -4.411 -11.456 1.00 15.00 ATOM 168 CG2 THR 134 -26.232 -4.411 -11.456 1.00 15.00 ATOM 169 C THR 134 -26.044 -2.897 -9.968 1.00 22.97 ATOM 169 C THR 134 -26.540 -5.037 -7.559 1.00 32.51 ATOM 170 O THR 134 -25.658 -3.461 -6.603 1.00 38.43 ATOM 171 N THR 135 -23.717 -3.352 -7.690 1.00 35.98 ATOM 172 H THR 135 -23.292 -3.555 -8.585 1.00 15.00 ATOM 173 CA THR 135 -22.964 -3.469 -6.386 1.00 36.02 ATOM 174 CB THR 135 -22.964 -3.469 -6.386 1.00 36.02 ATOM 175 HG1 THR 135 -22.2964 -3.469 -6.534 1.00 36.02 ATOM 175 HG1 THR 135 -22.2964 -7.488 1.00 30.60 ATOM 177 CG2 THR 135 -22.255 -6.094 -7.312 1.00 15.00 ATOM 177 CG2 THR 135 -22.256 -6.094 -7.312 1.00 35.55 ATOM 178 C THR 135 -22.266 -5.404 1.00 30.25 | | | | | | |
| ATOM 158 HZ2 LYS 133 -31.753 -8.299 -4.811 1.00 15.00 ATOM 159 HZ3 LYS 133 -31.333 -6.654 -4.760 1.00 15.00 ATOM 160 C LYS 133 -25.579 -6.876 -7.194 1.00 20.10 ATOM 161 O LYS 133 -24.378 -6.801 -7.007 1.00 17.94 ATOM 162 N THR 134 -26.260 -6.052 -7.983 1.00 22.95 ATOM 163 H THR 134 -27.275 -6.130 -8.036 1.00 15.00 ATOM 164 CA THR 134 -25.556 -4.879 -8.561 1.00 27.89 ATOM 165 CB THR 134 -26.498 -4.274 -9.592 1.00 24.59 ATOM 166 OG1 THR 134 -26.540 -5.037 -10.792 1.00 24.32 ATOM 167 HG1 THR 134 -26.232 -4.411 -11.456 1.00 15.00 ATOM 168 CG2 THR 134 -26.044 -2.897 -9.968 1.00 22.97 ATOM 169 C THR 134 -26.044 -2.897 -9.968 1.00 22.97 ATOM 169 C THR 134 -25.658 -3.461 -6.603 1.00 32.51 ATOM 170 O THR 134 -25.658 -3.461 -6.603 1.00 38.43 ATOM 171 N THR 135 -23.717 -3.352 -7.690 1.00 35.98 ATOM 172 H THR 135 -23.292 -3.555 -8.585 1.00 15.00 ATOM 173 CA THR 135 -22.964 -3.469 -6.386 1.00 36.02 ATOM 174 CB THR 135 -21.575 -4.276 -6.534 1.00 30.60 ATOM 175 GG1 THR 135 -22.964 -3.469 -6.386 1.00 30.60 ATOM 177 CG2 THR 135 -22.255 -6.094 -7.312 1.00 15.00 ATOM 177 CG2 THR 135 -22.255 -6.094 -7.312 1.00 35.55 ATOM 177 CG2 THR 135 -22.256 -5.404 1.00 30.25 | | | | | | |
| ATOM 159 HZ3 LYS 133 -31.333 -6.654 -4.760 1.00 15.00 ATOM 160 C LYS 133 -25.579 -6.876 -7.194 1.00 20.10 ATOM 161 O LYS 133 -24.378 -6.801 -7.007 1.00 17.94 ATOM 162 N THR 134 -26.260 -6.052 -7.983 1.00 22.95 ATOM 163 H THR 134 -27.275 -6.130 -8.036 1.00 15.00 ATOM 164 CA THR 134 -25.556 -4.879 -8.561 1.00 27.89 ATOM 165 CB THR 134 -26.498 -4.274 -9.592 1.00 24.59 ATOM 166 OG1 THR 134 -26.540 -5.037 -10.792 1.00 24.32 ATOM 167 HG1 THR 134 -26.044 -2.897 -9.968 1.00 22.97 ATOM 168 CG2 THR 134 -26.044 -2.897 -9.968 1.00 22.97 ATOM 169 C THR 134 -24.987 -3.798 -7.559 1.00 32.51 ATOM 170 O THR 134 -25.658 -3.461 -6.603 1.00 38.43 ATOM 171 N THR 135 -23.717 -3.352 -7.690 1.00 35.98 ATOM 172 H THR 135 -23.717 -3.352 -7.690 1.00 35.98 ATOM 173 CA THR 135 -22.2964 -3.469 -6.386 1.00 36.02 ATOM 174 CB THR 135 -21.575 -4.276 -6.534 1.00 30.60 ATOM 175 OG1 THR 135 -22.255 -6.094 -7.312 1.00 15.00 ATOM 176 HG1 THR 135 -22.255 -6.094 -7.312 1.00 15.00 ATOM 177 CG2 THR 135 -22.255 -6.094 -7.312 1.00 35.55 ATOM 177 CG2 THR 135 -22.255 -6.094 -7.312 1.00 35.55 | | | | | | |
| ATOM 160 C LYS 133 -25.579 -6.876 -7.194 1.00 20.10 ATOM 161 O LYS 133 -24.378 -6.801 -7.007 1.00 17.94 ATOM 162 N THR 134 -26.260 -6.052 -7.983 1.00 22.95 ATOM 163 H THR 134 -27.275 -6.130 -8.036 1.00 15.00 ATOM 164 CA THR 134 -25.556 -4.879 -8.561 1.00 27.89 ATOM 165 CB THR 134 -26.498 -4.274 -9.592 1.00 24.59 ATOM 166 OG1 THR 134 -26.540 -5.037 -10.792 1.00 24.32 ATOM 167 HG1 THR 134 -26.232 -4.411 -11.456 1.00 15.00 ATOM 168 CG2 THR 134 -26.044 -2.897 -9.968 1.00 22.97 ATOM 169 C THR 134 -24.987 -3.798 -7.559 1.00 32.51 ATOM 170 O THR 134 -25.658 -3.461 -6.603 1.00 38.43 ATOM 171 N THR 135 -23.717 -3.352 -7.690 1.00 35.98 ATOM 172 H THR 135 -23.717 -3.352 -7.690 1.00 35.98 ATOM 173 CA THR 135 -22.964 -3.469 -6.386 1.00 36.02 ATOM 174 CB THR 135 -22.964 -3.469 -6.386 1.00 36.02 ATOM 175 CG1 THR 135 -22.964 -7.312 1.00 30.60 ATOM 176 HG1 THR 135 -22.255 -6.094 -7.312 1.00 35.55 ATOM 177 CG2 THR 135 -22.255 -6.094 -7.312 1.00 35.55 ATOM 178 C THR 135 -22.949 -2.266 -5.404 1.00 30.25 | | | | | | |
| ATOM 161 O LYS 133 -24.378 -6.801 -7.007 1.00 17.94 ATOM 162 N THR 134 -26.260 -6.052 -7.983 1.00 22.95 ATOM 163 H THR 134 -27.275 -6.130 -8.036 1.00 15.00 ATOM 164 CA THR 134 -25.556 -4.879 -8.561 1.00 27.89 ATOM 165 CB THR 134 -26.498 -4.274 -9.592 1.00 24.59 ATOM 166 OG1 THR 134 -26.540 -5.037 -10.792 1.00 24.32 ATOM 167 HG1 THR 134 -26.232 -4.411 -11.456 1.00 15.00 ATOM 168 CG2 THR 134 -26.044 -2.897 -9.968 1.00 22.97 ATOM 169 C THR 134 -24.987 -3.798 -7.559 1.00 32.51 ATOM 170 O THR 134 -25.658 -3.461 -6.603 1.00 38.43 ATOM 171 N THR 135 -23.717 -3.352 -7.690 1.00 35.98 ATOM 172 H THR 135 -23.717 -3.352 -7.690 1.00 35.98 ATOM 173 CA THR 135 -22.964 -3.469 -6.386 1.00 36.02 ATOM 174 CB THR 135 -21.575 -4.276 -6.534 1.00 36.01 ATOM 175 OG1 THR 135 -21.575 -4.276 -6.534 1.00 36.01 ATOM 176 HG1 THR 135 -21.645 -5.388 -7.488 1.00 30.60 ATOM 177 CG2 THR 135 -22.255 -6.094 -7.312 1.00 15.00 ATOM 177 CG2 THR 135 -22.266 -5.404 1.00 35.55 ATOM 178 C THR 135 -22.949 -2.266 -5.404 1.00 30.25 | | | | | | |
| ATOM 162 N THR 134 -26.260 -6.052 -7.983 1.00 22.95 ATOM 163 H THR 134 -27.275 -6.130 -8.036 1.00 15.00 ATOM 164 CA THR 134 -25.556 -4.879 -8.561 1.00 27.89 ATOM 165 CB THR 134 -26.498 -4.274 -9.592 1.00 24.59 ATOM 166 OG1 THR 134 -26.540 -5.037 -10.792 1.00 24.32 ATOM 167 HG1 THR 134 -26.232 -4.411 -11.456 1.00 15.00 ATOM 168 CG2 THR 134 -26.044 -2.897 -9.968 1.00 22.97 ATOM 169 C THR 134 -24.987 -3.798 -7.559 1.00 32.51 ATOM 170 O THR 134 -25.658 -3.461 -6.603 1.00 38.43 ATOM 171 N THR 135 -23.717 -3.352 -7.690 1.00 35.98 ATOM 172 H THR 135 -23.292 -3.555 -8.585 1.00 15.00 ATOM 173 CA THR 135 -22.964 -3.469 -6.386 1.00 36.02 ATOM 174 CB THR 135 -21.575 -4.276 -6.534 1.00 36.01 ATOM 175 CG1 THR 135 -21.645 -5.388 -7.488 1.00 30.60 ATOM 176 HG1 THR 135 -22.255 -6.094 -7.312 1.00 15.00 ATOM 177 CG2 THR 135 -22.255 -6.094 -7.312 1.00 15.00 ATOM 177 CG2 THR 135 -22.266 -5.404 1.00 30.25 | | | | | | |
| ATOM 163 H THR 134 -27.275 -6.130 -8.036 1.00 15.00 ATOM 164 CA THR 134 -25.556 -4.879 -8.561 1.00 27.89 ATOM 165 CB THR 134 -26.498 -4.274 -9.592 1.00 24.59 ATOM 166 OG1 THR 134 -26.540 -5.037 -10.792 1.00 24.32 ATOM 167 HG1 THR 134 -26.232 -4.411 -11.456 1.00 15.00 ATOM 168 CG2 THR 134 -26.044 -2.897 -9.968 1.00 22.97 ATOM 169 C THR 134 -24.987 -3.798 -7.559 1.00 32.51 ATOM 170 O THR 134 -25.658 -3.461 -6.603 1.00 38.43 ATOM 171 N THR 135 -23.717 -3.352 -7.690 1.00 35.98 ATOM 172 H THR 135 -23.717 -3.352 -7.690 1.00 35.98 ATOM 173 CA THR 135 -22.964 -3.469 -6.386 1.00 36.02 ATOM 174 CB THR 135 -22.964 -3.469 -6.386 1.00 36.01 ATOM 175 OG1 THR 135 -21.575 -4.276 -6.534 1.00 36.01 ATOM 176 HG1 THR 135 -22.255 -6.094 -7.312 1.00 15.00 ATOM 177 CG2 THR 135 -22.255 -6.094 -7.312 1.00 15.00 ATOM 177 CG2 THR 135 -22.2949 -2.266 -5.404 1.00 30.25 ATOM 178 C THR 135 -22.949 -2.266 -5.404 1.00 30.25 | | | | | | |
| ATOM 164 CA THR 134 -25.556 -4.879 -8.561 1.00 27.89 ATOM 165 CB THR 134 -26.498 -4.274 -9.592 1.00 24.59 ATOM 166 OG1 THR 134 -26.540 -5.037 -10.792 1.00 24.32 ATOM 167 HG1 THR 134 -26.232 -4.411 -11.456 1.00 15.00 ATOM 168 CG2 THR 134 -26.044 -2.897 -9.968 1.00 22.97 ATOM 169 C THR 134 -24.987 -3.798 -7.559 1.00 32.51 ATOM 170 O THR 134 -25.658 -3.461 -6.603 1.00 38.43 ATOM 171 N THR 135 -23.717 -3.352 -7.690 1.00 35.98 ATOM 172 H THR 135 -23.292 -3.555 -8.585 1.00 15.00 ATOM 173 CA THR 135 -22.964 -3.469 -6.386 1.00 36.02 ATOM 174 CB THR 135 -21.575 -4.276 -6.534 1.00 36.01 ATOM 175 OG1 THR 135 -21.645 -5.388 -7.488 1.00 30.60 ATOM 176 HG1 THR 135 -22.255 -6.094 -7.312 1.00 15.00 ATOM 177 CG2 THR 135 -22.255 -6.094 -7.312 1.00 15.00 ATOM 178 C THR 135 -22.969 -2.266 -5.404 1.00 30.25 | | | | | | |
| ATOM 165 CB THR 134 -26.498 -4.274 -9.592 1.00 24.59 ATOM 166 OG1 THR 134 -26.540 -5.037 -10.792 1.00 24.32 ATOM 167 HG1 THR 134 -26.232 -4.411 -11.456 1.00 15.00 ATOM 168 CG2 THR 134 -26.044 -2.897 -9.968 1.00 22.97 ATOM 169 C THR 134 -24.987 -3.798 -7.559 1.00 32.51 ATOM 170 O THR 134 -25.658 -3.461 -6.603 1.00 38.43 ATOM 171 N THR 135 -23.717 -3.352 -7.690 1.00 35.98 ATOM 172 H THR 135 -23.717 -3.352 -7.690 1.00 35.98 ATOM 173 CA THR 135 -23.292 -3.555 -8.585 1.00 15.00 ATOM 174 CB THR 135 -22.964 -3.469 -6.386 1.00 36.02 ATOM 175 OG1 THR 135 -21.575 -4.276 -6.534 1.00 36.01 ATOM 176 HG1 THR 135 -21.645 -5.388 -7.488 1.00 30.60 ATOM 177 CG2 THR 135 -22.255 -6.094 -7.312 1.00 15.00 ATOM 178 C THR 135 -22.949 -2.266 -5.404 1.00 30.25 | | | | | | |
| ATOM 166 OG1 THR 134 -26.540 -5.037 -10.792 1.00 24.32 ATOM 167 HG1 THR 134 -26.232 -4.411 -11.456 1.00 15.00 ATOM 168 CG2 THR 134 -26.044 -2.897 -9.968 1.00 22.97 ATOM 169 C THR 134 -24.987 -3.798 -7.559 1.00 32.51 ATOM 170 O THR 134 -25.658 -3.461 -6.603 1.00 38.43 ATOM 171 N THR 135 -23.717 -3.352 -7.690 1.00 35.98 ATOM 172 H THR 135 -23.292 -3.555 -8.585 1.00 15.00 ATOM 173 CA THR 135 -22.964 -3.469 -6.386 1.00 36.02 ATOM 174 CB THR 135 -21.575 -4.276 -6.534 1.00 36.01 ATOM 175 OG1 THR 135 -21.645 -5.388 -7.488 1.00 30.60 ATOM 176 HG1 THR 135 -22.255 -6.094 -7.312 1.00 15.00 ATOM 177 CG2 THR 135 -20.866 -4.776 -5.264 1.00 35.55 ATOM 178 C THR 135 -22.949 -2.266 -5.404 1.00 30.25 | | | | | | |
| ATOM 167 HG1 THR 134 -26.232 -4.411 -11.456 1.00 15.00 ATOM 168 CG2 THR 134 -26.044 -2.897 -9.968 1.00 22.97 ATOM 169 C THR 134 -24.987 -3.798 -7.559 1.00 32.51 ATOM 170 O THR 134 -25.658 -3.461 -6.603 1.00 38.43 ATOM 171 N THR 135 -23.717 -3.352 -7.690 1.00 35.98 ATOM 172 H THR 135 -23.292 -3.555 -8.585 1.00 15.00 ATOM 173 CA THR 135 -22.964 -3.469 -6.386 1.00 36.02 ATOM 174 CB THR 135 -21.575 -4.276 -6.534 1.00 36.01 ATOM 175 OG1 THR 135 -21.645 -5.388 -7.488 1.00 30.60 ATOM 176 HG1 THR 135 -22.255 -6.094 -7.312 1.00 15.00 ATOM 177 CG2 THR 135 -20.866 -4.776 -5.264 1.00 35.55 ATOM 178 C THR 135 -22.949 -2.266 -5.404 1.00 30.25 | | | | | | |
| ATOM 168 CG2 THR 134 -26.044 -2.897 -9.968 1.00 22.97 ATOM 169 C THR 134 -24.987 -3.798 -7.559 1.00 32.51 ATOM 170 O THR 134 -25.658 -3.461 -6.603 1.00 38.43 ATOM 171 N THR 135 -23.717 -3.352 -7.690 1.00 35.98 ATOM 172 H THR 135 -23.292 -3.555 -8.585 1.00 15.00 ATOM 173 CA THR 135 -22.964 -3.469 -6.386 1.00 36.02 ATOM 174 CB THR 135 -21.575 -4.276 -6.534 1.00 36.01 ATOM 175 OG1 THR 135 -21.645 -5.388 -7.488 1.00 30.60 ATOM 176 HG1 THR 135 -22.255 -6.094 -7.312 1.00 15.00 ATOM 177 CG2 THR 135 -20.866 -4.776 -5.264 1.00 35.55 ATOM 178 C THR 135 -22.949 -2.266 -5.404 1.00 30.25 | | | | | | |
| ATOM 169 C THR 134 -24.987 -3.798 -7.559 1.00 32.51 ATOM 170 O THR 134 -25.658 -3.461 -6.603 1.00 38.43 ATOM 171 N THR 135 -23.717 -3.352 -7.690 1.00 35.98 ATOM 172 H THR 135 -23.292 -3.555 -8.585 1.00 15.00 ATOM 173 CA THR 135 -22.964 -3.469 -6.386 1.00 36.02 ATOM 174 CB THR 135 -21.575 -4.276 -6.534 1.00 36.01 ATOM 175 OG1 THR 135 -21.645 -5.388 -7.488 1.00 30.60 ATOM 176 HG1 THR 135 -22.255 -6.094 -7.312 1.00 15.00 ATOM 177 CG2 THR 135 -20.866 -4.776 -5.264 1.00 35.55 ATOM 178 C THR 135 -22.949 -2.266 -5.404 1.00 30.25 | | | | | | |
| ATOM 170 O THR 134 -25.658 -3.461 -6.603 1.00 38.43 ATOM 171 N THR 135 -23.717 -3.352 -7.690 1.00 35.98 ATOM 172 H THR 135 -23.292 -3.555 -8.585 1.00 15.00 ATOM 173 CA THR 135 -22.964 -3.469 -6.386 1.00 36.02 ATOM 174 CB THR 135 -21.575 -4.276 -6.534 1.00 36.01 ATOM 175 OG1 THR 135 -21.645 -5.388 -7.488 1.00 30.60 ATOM 176 HG1 THR 135 -22.255 -6.094 -7.312 1.00 15.00 ATOM 177 CG2 THR 135 -20.866 -4.776 -5.264 1.00 35.55 ATOM 178 C THR 135 -22.949 -2.266 -5.404 1.00 30.25 | | | | | | |
| ATOM 171 N THR 135 -23.717 -3.352 -7.690 1.00 35.98 ATOM 172 H THR 135 -23.292 -3.555 -8.585 1.00 15.00 ATOM 173 CA THR 135 -22.964 -3.469 -6.386 1.00 36.02 ATOM 174 CB THR 135 -21.575 -4.276 -6.534 1.00 36.01 ATOM 175 OG1 THR 135 -21.645 -5.388 -7.488 1.00 30.60 ATOM 176 HG1 THR 135 -22.255 -6.094 -7.312 1.00 15.00 ATOM 177 CG2 THR 135 -20.866 -4.776 -5.264 1.00 35.55 ATOM 178 C THR 135 -22.949 -2.266 -5.404 1.00 30.25 | | | | | | |
| ATOM 172 H THR 135 -23.292 -3.555 -8.585 1.00 15.00 ATOM 173 CA THR 135 -22.964 -3.469 -6.386 1.00 36.02 ATOM 174 CB THR 135 -21.575 -4.276 -6.534 1.00 36.01 ATOM 175 OG1 THR 135 -21.645 -5.388 -7.488 1.00 30.60 ATOM 176 HG1 THR 135 -22.255 -6.094 -7.312 1.00 15.00 ATOM 177 CG2 THR 135 -20.866 -4.776 -5.264 1.00 35.55 ATOM 178 C THR 135 -22.949 -2.266 -5.404 1.00 30.25 | | | | | | |
| ATOM 173 CA THR 135 -22.964 -3.469 -6.386 1.00 36.02 ATOM 174 CB THR 135 -21.575 -4.276 -6.534 1.00 36.01 ATOM 175 OG1 THR 135 -21.645 -5.388 -7.488 1.00 30.60 ATOM 176 HG1 THR 135 -22.255 -6.094 -7.312 1.00 15.00 ATOM 177 CG2 THR 135 -20.866 -4.776 -5.264 1.00 35.55 ATOM 178 C THR 135 -22.949 -2.266 -5.404 1.00 30.25 | | -/1 | | | | |
| ATOM 174 CB THR 135 -21.575 -4.276 -6.534 1.00 36.01 ATOM 175 OG1 THR 135 -21.645 -5.388 -7.488 1.00 30.60 ATOM 176 HG1 THR 135 -22.255 -6.094 -7.312 1.00 15.00 ATOM 177 CG2 THR 135 -20.866 -4.776 -5.264 1.00 35.55 ATOM 178 C THR 135 -22.949 -2.266 -5.404 1.00 30.25 | | | | | | |
| ATOM 175 OG1 THR 135 -21.645 -5.388 -7.488 1.00 30.60 ATOM 176 HG1 THR 135 -22.255 -6.094 -7.312 1.00 15.00 ATOM 177 CG2 THR 135 -20.866 -4.776 -5.264 1.00 35.55 ATOM 178 C THR 135 -22.949 -2.266 -5.404 1.00 30.25 | | | | | | |
| ATOM 176 HG1 THR 135 -22.255 -6.094 -7.312 1.00 15.00 ATOM 177 CG2 THR 135 -20.866 -4.776 -5.264 1.00 35.55 ATOM 178 C THR 135 -22.949 -2.266 -5.404 1.00 30.25 | | | | | | |
| ATOM 177 CG2 THR 135 -20.866 -4.776 -5.264 1.00 35.55 ATOM 178 C THR 135 -22.949 -2.266 -5.404 1.00 30.25 | | | | | | |
| ATOM 178 C THR 135 -22.949 -2.266 -5.404 1.00 30.25 | | | | | | |
| ALOM 170 C THE 177 | | | | | 4 4 5 | |
| ATOM 1/9 0 1HK 135 -23.541 -2.346 -4.331 1.00 20.33 | | | | | | |
| | ATOM | 179 | ن ت | HR | - 72 | -72.241 -7.240 4.221 1.00 20.22 |

FIGURE 17D

| ATOM | 180 | N | SER | 136 | -22.294 | -1.146 | -5.776 | | |
|--------|-----|------|-----|-------|---------|----------------|--------|------------|-----|
| ATOM | 181 | | SER | 136 | -22.828 | -0.357 | -5.460 | 1.00 23.2 | |
| MCTA | 182 | | SER | 136 | -20.857 | -1.051 | | | |
| ATOM | 183 | | SER | 136 | | | -6.143 | 1.00 23.0 | |
| | | | | | -20.560 | 0.187 1.261 | -6.965 | 1.00 21.0 | |
| ATOM | 184 | | SER | 136 | -20.624 | | -6.043 | 1.00 28.2 | |
| ATOM | 185 | | SER | 136 | -19.815 | 1.793 | -6.008 | 1.00 15.0 | |
| ATOM | 186 | | SER | 136 | -19.853 | -1.090 | -4.958 | 1.00 21.7 | |
| ATOM | 187 | | SER | 136 | -18.630 | -1.096 | -5.080 | 1.00 21.9 | 4 A |
| MOTA | 188 | N | VAL | 137 | -20.452 | -1.227 | -3.752 | 1.00 24.0 | 3 A |
| ATOM | 189 | H | VAL | 137 | -21.440 | -1.063 | -3.705 | 1.00 15.0 | 0 A |
| ATOM | 190 | CA | VAL | 137 | -19.699 | -1.632 | -2.570 | 1.00 19.6 | 5 A |
| ATOM | 191 | CB | VAL | 137 | -20.218 | -1.010 | -1.248 | 1.00 21.1 | |
| ATOM | 192 | CG1 | VAL | 137 | -20.419 | -1.907 | -0.058 | 1.00 18.1 | 6 A |
| ATOM | 193 | CG2 | VAL | 137 | -21.322 | -0.026 | -1.442 | 1.00 13.4 | |
| ATOM | 194 | С | VAL | 137 | -19.370 | -3.116 | -2.473 | 1.00 17.1 | |
| ATOM | 195 | ō | VAL | 137 | -20.209 | -3.969 | -2.593 | 1.00 16.6 | |
| ATOM | 196 | N | LEU | 138 | -18.077 | -3.344 | -2.271 | 1.00 15.8 | |
| ATOM | 197 | н | LEU | 138 | -17.502 | -2.528 | -2.246 | 1.00 15.0 | |
| ATOM | 198 | CA | LEU | 138 | -17.507 | -4.667 | -1.938 | | |
| ATOM | 199 | CB | | 138 | -15.962 | | | | |
| | | | LEU | | | -4.530 | -1.791 | 1.00 13.60 | |
| ATOM | 200 | CG | LEU | 138 | -15.273 | -3.854 | -2.998 | 1.00 16.09 | |
| ATOM | 201 | | LEU | 138 | -15.923 | -4.379 | -4.300 | 1.00 20.3 | |
| ATOM | 202 | CD2 | LEU | 138 | -13.710 | -3.936 | -2.982 | 1.00 12.34 | |
| ATOM | 203 | C | LEU | 138 | -18.170 | -5.480 | -0.772 | 1.00 16.29 | |
| ATOM | 204 | 0 | LEU | 138 | -18.498 | -4.986 | 0.301 | 1.00 12.97 | |
| ATOM | 205 | N | GLN | 139 | -18.345 | -6.768 | -1.035 | 1.00 13.04 | A A |
| ATOM | 206 | H | GLN | 139 | -18.052 | -7.078 | -1.960 | 1.00 15.00 |) A |
| ATOM | 207 | CA | GLN | 139 | -18.757 | -7.658 | 0.013 | 1.00 15.32 | 2 A |
| ATOM | 208 | CB | GLN | 139 | -19.847 | -8.678 | -0.481 | 1.00 13.99 | |
| MOTA | 209 | CG | GLN | 139 | -21.068 | -7.960 | -1.113 | 1.00 20.85 | |
| ATOM | 210 | CD | GLN | 139 | -21.872 | -7.022 | -0.193 | 1.00 22.04 | |
| ATOM | 211 | OE1 | GLN | 139 | -22.343 | -7.439 | 0.878 | 1.00 25.45 | |
| ATOM | 212 | NE2 | GLN | 139 | -21.963 | -5.739 | -0.618 | 1.00 17.74 | |
| ATOM | 213 | HE21 | | 139 | -22.697 | -5.181 | -0.206 | 1.00 15.00 | |
| MOTA | 214 | HE22 | GLN | 139 | -21.460 | -5.326 | -1.374 | 1.00 15.00 | |
| ATOM | 215 | C | GLN | 139 | -17.527 | -8.383 | 0.541 | 1.00 14.26 | |
| ATOM | 216 | Ö | GLN | 139 | -16.554 | -8.640 | -0.144 | 1.00 14.40 | |
| MCTA | 217 | N | TRP | 140 | -17.647 | -8.780 | 1.805 | 1.00 12.80 | |
| ATOM | 218 | H | TRP | 140 | -18.433 | -8.447 | 2.297 | 1.00 15.00 | |
| ATOM | 219 | CA | TRP | 140 | -16.542 | -9.500 | 2.463 | | |
| MCTA | 220 | CB | TRP | 140 | -15.813 | | | 1.00 14.03 | |
| ATOM | 221 | CG | TRP | 140 | | -8.623 | 3.483 | 1.00 14.18 | |
| | | | | | -15.467 | -7.291 | 2.823 | 1.00 8.44 | |
| ATOM | 222 | CD2 | TRP | 140 | -14.379 | -6.966 | 1.941 | 1.00 9.01 | |
| ATOM | 223 | CE2 | TRP | 140 | -14.549 | -5.625 | 1.482 | 1.00 8.40 | |
| ATOM | 224 | | TRP | 140 | -13.215 | -7.688 | 1.581 | 1.00 10.14 | |
| MOTA | 225 | | TRP | 140 | -16.225 | -6.137 | 2.863 | 1.00 11.29 | |
| ATOM | 226 | NEI | TRP | 140 | -15.710 | -5.150 | 2.077 | 1.00 14.27 | |
| ATOM | 227 | HE1 | TRP | 140 | -16.121 | -4.268 | 2.010 | 1.00 15.00 |) A |
| ATOM | 228 | CZ2 | TRP | 140 | -13.640 | -5.009 | 0.590 | 1.00 8.16 | |
| ATOM | 229 | CZ3 | TRP | 140 | -12.292 | -7.069 | 0.713 | 1.00 13.90 |) A |
| ATOM | 230 | CH2 | TRP | 140 | -12.497 | -5.749 | 0.215 | 1.00 12.11 | . А |
| ATOM | 231 | C | TRP | 140 | | -10.701 | 3.170 | 1.00 14.34 | |
| ATOM | 232 | 0 | TRP | 140 | -18.193 | -10.862 | 3.392 | 1.00 16.00 | |
| ATOM ' | 233 | N | ALA | 141 | | -11.528 | 3.558 | 1.00 14.80 | |
| ATOM | 234 | н | ALA | 141 | | -11.377 | 3.294 | 1.00 15.00 | |
| ATOM | 235 | CA | ALA | 141 | -16.489 | -12.617 | 4.394 | 1.00 15.27 | |
| ATOM | 236 | CB | ALA | 141 | | -13.920 | 3.583 | 1.00 16.97 | |
| ATOM | 237 | Ē | ALA | 141 | | -12.761 | 5.607 | 1.00 15.90 | |
| ATOM | 239 | Ö | ALA | 141 | -14.453 | -12.338 | 5.550 | 1.00 14.25 | |
| ATOM | 239 | Ŋ | GLU | 142 | | -13.366 | 6.688 | 1.00 19.74 | |
| | | •• | J_5 | 4 1 4 | 20.000 | 13.300 | 5.555 | 2.00 19.79 | ^ |

FIGURE 17E

| 101014 | 240 | | ~ | | | | | | |
|--------|-----|--------------|-----|------------------|--------|------------|----------|----------|------------------|
| ATOM | 240 | H | GLU | 142 | -17.0 | 55 -13.574 | 6.688 | | .00 % |
| ATOM | 241 | ÇA | GLU | 142 | -15.14 | 9 -13.759 | 7.731 | 1.00 25 | . 9 3 |
| ATOM | 242 | CB | GLU | 142 | -15.79 | 4 -13.910 | 9.117 | | .75 |
| ATOM | 243 | CG | GLU | 142 | -15.73 | | | | |
| | | | | | | | | | .05 |
| ATOM | 244 | CD | GLU | 142 | -16.74 | | 7 10.711 | 1.00 26 | .61 |
| ATOM | 245 | OE1 | GLU | 142 | -17.90 | 8 -11.888 | 3 10.361 | 1.00 34 | .72 p |
| ATOM | 246 | OE2 | GLU | 142 | -16.40 | 4 -11.984 | 11.886 | | . סלס |
| ATOM | 247 | c | GLU | 142 | -14.20 | | | | |
| | | | | | | | | 1.00 33 | |
| ATCM | 248 | 0 | GLU | 142 | | 6 -14.349 | | 1.00 41 | .84 A |
| ATOM | 249 | N | LYS | 143 | -14.57 | 7 -16.080 | 7.084 | 1.00 34. | |
| ATOM | 250 | Н | LYS | 143 | -15.43 | 2 -16.384 | 7.492 | 1.00 15. | |
| ATOM | 251 | CA | LYS | 143 | | 2 -16.854 | | 1.00 35. | _ |
| | | | | | | | | | |
| ATOM | 252 | CB | LYS | 143 | -14.67 | | | 1.00 37. | .64 A |
| ATOM | 253 | CG | LYS | 143 | -14.30 | 0 -17.505 | 3.531 | 1.00 47. | .37 A |
| ATOM | 254 | CD | LYS | 143 | -15.02 | 2 -17.284 | 2.202 | 1.00 50. | .37 A |
| ATOM | 255 | CE | LYS | 143 | -14.68 | | | 1.00 49. | |
| | | | | | | | | | |
| ATOM | 256 | NZ | LYS | 143 | -15.63 | | | 1.00 51. | |
| ATOM | 257 | HZ1 | | 143 | -15.33 | | | 1.00 15. | 00 A |
| ATOM | 258 | HZ2 | LYS | 143 | -15.68 | 0 -17.061 | -0.177 | 1.00 15. | 00 A |
| ATOM | 259 | HZ3 | LYS | 143 | -16.56 | 415.833 | 0.585 | 1.00 15. | |
| ATOM | 260 | C | LYS | 143 | -12.33 | | | | |
| | | | | | | | | 1.00 32. | |
| ATOM | 261 | 0 | LYS | 143 | | 1 -18.041 | | 1.00 35. | |
| ATOM | 262 | N | GLY | 144 | -11.52 | 2 -15.923 | 5.637 | 1.00 28. | 26 A |
| ATOM | 263 | H | GLY | 144 | -11.71 | 8 -14.995 | 5.910 | 1.00 15. | |
| ATOM | 264 | CA | GLY | 144 | -10.24 | | | 1.00 32. | |
| ATOM | 265 | | GLY | 144 | -9.17 | | | | |
| | | C | | | | | | 1.00 29. | |
| ATOM | 266 | 0 | GLY | 144 | -9.34 | | | 1.00 24. | - |
| MCTA | 267 | N | TYR | 145 | -8.06 | 9 -16.270 | 5.815 | 1.00 26. | 37 A |
| ATOM | 268 | Н | TYR | 145 | -8.16 | 0 -15.729 | 4.966 | 1.00 15. | |
| ATOM | 269 | CA | TYR | 145 | -7.02 | | 6.777 | 1.00 27. | |
| | | | TYR | | | | | | |
| ATOM | 270 | CB | | 145 | -5.70 | | 5.947 | 1.00 37. | |
| ATOM | 271 | CG | TYR | 145 | -5.96 | | 4.456 | 1.00 50. | 95 A |
| ATOM | 272 | CD1 | TYR | 145 | -5.68 | 2 -14.633 | 3.706 | 1.00 53. | 22 A |
| ATOM | 273 | CE1 | TYR | 145 | -6.31 | 3 -14.377 | 2.468 | 1.00 60. | |
| ATOM | 274 | CD2 | TYR | 145 | -6.59 | | 3.791 | 1.00 53. | |
| | | | | | | | | | |
| ATOM | 275 | CE2 | TYR | 145 | -7.20 | | | 1.00 56. | |
| ATOM | 276 | CZ | TYR | 145 | -7.16 | 2 -15.430 | 1.873 | 1.00 61. | 12 A |
| ATOM | 277 | OH | TYR | 145 | -7.81 | 2 -15.119 | 0.665 | 1.00 62. | 63 A |
| ATOM | 278 | HH | TYR | 145 | -8.57 | 5 -15.686 | 0.401 | 1.00 15. | |
| ATOM | 279 | C | TYR | 145 | -7.53 | | 7.620 | 1.00 22. | |
| ATOM | | | | | | | | | |
| | 280 | 0 | TYR | 145 | -7.00 | | 7.650 | 1.00 22. | |
| MOTA | 281 | N | TYR | 146 | -8.73 | | 8.196 | 1.00 20. | |
| ATOM | 282 | Н | TYR | 146 | -8.93 | 5 -15.824 | 8.509 | 1.00 15. | 00 A |
| ATOM | 283 | CA | TYR | 146 | -9.42 | 3 -13.700 | 8.725 | 1.00 20. | 40 A |
| ATOM | 284 | CB | TYR | 146 | | 6 -13.673 | 8.306 | 1.00 22. | |
| | | | | | | | | | |
| | 285 | CG | TYR | 146 | | 0 -14.460 | 9.286 | 1.00 23. | |
| ATOM | 286 | CD1 | TYR | 146 | | 5 -15.873 | 9.236 | 1.00 26. | 99 A |
| ATOM | 287 | CE1 | TYR | 146 | -12.25 | 4 -16.623 | 10.239 | 1.00 25. | 44 A |
| ATOM | 288 | CD2 | TYR | 146 | -12.47 | 7 -13.766 | 10.236 | 1.00 23. | |
| ATOM | 289 | CE2 | TYR | 146 | | 0 -14.520 | | 1.00 26. | |
| | | | | | | | | | |
| ATOM | 290 | CZ | TYR | 146 | | 7 -15.937 | | 1.00 27. | |
| ATOM | 291 | ОН | TYR | 146 | | 7 -16.689 | 12.170 | 1.00 31. | |
| MOTA | 292 | HH | TYR | 146 | -12.91 | 1 -17.080 | 12.676 | 1.00 15. | 00 A |
| ATOM | 293 | C | TYR | 146 | -9.29 | 1 -13.419 | | 1.00 18. | |
| ATOM | 294 | Š | TYR | 146 | -8.90 | | 11.012 | 1.00 16. | |
| ATOM | 295 | N | THR | 147 | -9.59 | | | 1.00 17. | |
| | | | | | | | | | |
| MOTA | 296 | Н | THR | 147 | -9.97 | | | 1.00 15. | |
| ATOM | 297 | CA | THR | 147 | -9.43 | 2 -11.764 | 11.948 | 1.00 14. | 06 A |
| MCTA | 298 | CB | THR | 147 | -8.16 | 2 -10.875 | 12.182 | 1.00 13. | 66 A |
| MCTA | 299 | 0 G 1 | | 147 | | 2 -11.505 | | 1.00 12. | |
| | | | | - - · | J. 7 L | | | | ^ |

FIGURE 17F

| ATOM | 300 HG1 | THR | 147 | -6.934 | -11.898 | 10.980 | 1.00 15.00 |
|------|----------|-----|-----|---------|---------|--------|------------|
| | | THR | 147 | -8.025 | -10.236 | 13.554 | 1.00 7.22 |
| ATOM | 301 CG2 | | | | -10.925 | 12.253 | 1.00 15.60 |
| ATOM | 302 C | THR | 147 | | | | |
| ATOM | 303 0 | THR | 147 | -11.044 | -10.074 | 11.496 | 1.00 16.39 |
| | 304 N | MET | 148 | -11.144 | -11.139 | 13.412 | 1.00 20.67 |
| MOTA | | | 148 | | -11.988 | 13.828 | 1.00 15.00 |
| ATOM | 305 H | MET | | _ | | | |
| ATOM | 306 CA | MET | 148 | | -10.311 | 14.110 | 1.00 19.71 |
| ATOM | 307 CB | MET | 148 | -13.546 | -10.702 | 13.705 | 1.00 17.89 |
| | | MET | 148 | -14.541 | -9.580 | 14.019 | 1.00 13.53 |
| ATOM | 308 CG | | | | -8.149 | 12.952 | 1.00 14.69 |
| ATOM | 309 SD | MET | 148 | -14.492 | | | |
| ATOM | 310 CE | MET | 148 | -14.566 | -8.928 | 11.333 | 1.00 10.10 |
| ATOM | 311 C | MET | 148 | -11.915 | -10.282 | 15.639 | 1.00 21.49 |
| | | MET | 148 | -12.594 | -10.905 | 16.436 | 1.00 22.98 |
| ATOM | 312 0 | | | -10.955 | -9.412 | 16.055 | 1.00 20.58 |
| MOTA | 313 N | SER | 149 | | | | |
| ATOM | 314 H | SER | 149 | -10.516 | -8.786 | 15.406 | 1.00 15.00 |
| ATOM | 315 CA | SER | 149 | -10.388 | -9.698 | 17.419 | 1.00 19.11 |
| | | | 149 | -9.174 | -8.860 | 17.792 | 1.00 12.17 |
| ATOM | 316 CB | SER | | | | 17.975 | 1.00 14.10 |
| ATOM | 317 OG | SER | 149 | -9.540 | -7.513 | | |
| ATOM | 318 HG | SER | 149 | -9.571 | -7.487 | 18.934 | 1.00 15.00 |
| MOTA | 319 C | SER | 149 | -11.203 | -9.844 | 18.727 | 1.00 22.19 |
| | | | 149 | | -10.267 | 19.772 | 1.00 22.95 |
| ATOM | 320 O | SER | | | -9.322 | 18.631 | 1.00 22.71 |
| ATOM | 321 N | asn | 150 | -12.456 | | | |
| MOTA | 322 H | ASN | 150 | -12.782 | -9.247 | 17.688 | 1.00 15.00 |
| | 323 CA | ASN | 150 | -13.361 | -9.236 | 19.764 | 1.00 20.32 |
| ATOM | | ASN | 150 | -12.734 | -8.446 | 20.955 | 1.00 21.56 |
| ATOM | 324 CB | | | | - | 20.706 | 1.00 20.71 |
| ATOM | 325 CG | ASN | 150 | -12.343 | -6.962 | | |
| ATOM | 326 OD1 | ASN | 150 | -13.059 | -6.187 | 20.119 | 1.00 17.81 |
| | 327 ND2 | ASN | 150 | -11.222 | -6.485 | 21.271 | 1.00 23.86 |
| MOTA | | | 150 | -11.035 | -5.521 | 21.092 | 1.00 15.00 |
| ATOM | 328 HD21 | | | | | | 1.00 15.00 |
| ATOM | 329 HD22 | ASN | 150 | -10.670 | -7.109 | 21.821 | |
| ATOM | 330 C | ASN | 150 | -14.644 | -8.657 | 19.256 | 1.00 20.60 |
| | | ASN | 150 | -14.718 | -8.130 | 18.148 | 1.00 20.56 |
| ATOM | | | | -15.637 | -8.713 | 20.149 | 1.00 23.49 |
| MOTA | 332 N | NZA | 151 | | - | | 1.00 15.00 |
| ATOM | 333 H | ASN | 151 | -15.455 | -9.124 | 21.038 | |
| ATOM | 334 CA | ASN | 151 | -16.974 | -8.080 | 19.823 | 1.00 24.71 |
| | 335 CB | ASN | 151 | -18.130 | -8.645 | 20.712 | 1.00 28.30 |
| ATOM | | | | -17.959 | -8.271 | 22.173 | 1.00 33.23 |
| MOTA | 336 CG | ASN | 151 | | | 22.606 | 1.00 39.79 |
| MOTA | 337 OD1 | ASN | 151 | -17.075 | -7.562 | | _ |
| ATOM | 338 ND2 | ASN | 151 | -18.782 | -8.838 | 23.011 | 1.00 38.32 |
| | 339 HD21 | | 151 | -18.553 | -8.524 | 23.928 | 1.00 15.00 |
| ATOM | | | 151 | -19.495 | -9.465 | 22.733 | 1.00 15.00 |
| MCTA | 340 HD22 | ASN | | | | 19.645 | 1.00 22.53 |
| ATOM | 341 C | ASN | 151 | -17.172 | -6.531 | | |
| MOTA | 342 0 | ASN | 151 | -18.254 | -6.048 | 19.374 | 1.00 21.32 |
| ATOM | 343 N | LEU | 152 | -16.066 | -5.762 | 19.859 | 1.00 23.00 |
| | - | | 152 | -15.247 | -6.289 | 20.070 | 1.00 15.00 |
| ATOM | 344 H | LEU | | | -4.335 | 19.525 | 1.00 18.87 |
| MCTA | 345 CA | LEU | 152 | -15.924 | | | |
| ATOM | 346 CB | LEU | 152 | -14.830 | -3.700 | 20.325 | 1.00 21.77 |
| | 347 CG | LEU | 152 | -14.981 | -3.999 | 21.806 | 1.00 24.80 |
| MOTA | | | 152 | -16.390 | -3.645 | 22.316 | 1.00 22.82 |
| MOTA | | LEU | | | | 22.556 | 1.00 23.56 |
| ATOM | 349 CD2 | LEU | 152 | -13.847 | -3.256 | | |
| ATOM | 350 C | LEU | 152 | -15.565 | -3.993 | 18.094 | 1.00 17.34 |
| ATOM | 351 0 | LEU | 152 | -15.590 | -2.840 | 17.708 | 1.00 13.39 |
| | | | 153 | -15.267 | -5.054 | 17.309 | 1.00 18.65 |
| ATOM | 352 N | VAL | | | -5.962 | 17.716 | 1.00 15.00 |
| ATOM | 353 H | VAL | 153 | -15.156 | | | |
| MCTA | 354 CA | VAL | 153 | -15.439 | -4.910 | 15.849 | 1.00 16.81 |
| ATOM | 355 CB | VAL | 153 | -14.138 | -5.021 | 14.980 | 1.00 15.33 |
| | | | 153 | -12.908 | -5.718 | 15.562 | 1.00 21.22 |
| ATOM | | | | -13.775 | -3.757 | 14.287 | 1.00 16.95 |
| ATOM | 357 CG2 | | 153 | | | | 1.00 13.48 |
| ATOM | 358 C | VAL | 153 | -16.405 | -5.964 | 15.301 | |
| ATOM | 359 0 | VAL | 153 | -16.363 | -7.116 | 15.647 | 1.00 13.06 |
| | | | | | | | |

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FIGURE 17G

| ATOM | 360 | N | THR | .154 | -17.207 | -5.546 | 14.358 | 1.00 12.06 |
|------|------------|-----------|------|------|--------------------|---------|--------|-------------|
| | 361 | H | THR | 154 | -17.313 | -4.568 | 14.215 | 1.00 15.00 |
| ATOM | 36.2 | CA | THR | 154 | -17.903 | -6.600 | 13.615 | 1.00 16.26 |
| ATOM | 363 | CB | THR | 154 | -19.366 | -6.747 | 14.157 | 1.00 19.51 |
| ATOM | | OG1 | THR | 154 | -19.995 | -5.459 | 14.205 | 1.00 19.31 |
| ATOM | 364 | | THR | 154 | -20.577 | -5.508 | 14.949 | 1.00 15.00 |
| ATOM | 365 | HG1 | | | -19.502 | -7:288 | 15.571 | 1.00 21.62 |
| ATOM | 366 | CG2 | THR | 154 | -17.997 | -6.252 | 12.107 | 1.00 18.12 |
| MOTA | 367 | C | THR | 154 | -17.992 | -5.110 | 11.605 | 1.00 16.55 |
| ATOM | 368 | 0 | THR | 154 | -18.101 | -7.324 | 11.357 | 1.00 16.77 |
| ATOM | 369 | N | LEU | 155 | -18.056 | -8.202 | 11.791 | 1.00 15.00 |
| ATOM | 370 | H | LEU | 155 | -18.514 | -7.198 | 9.967 | 1.00 17.10 |
| MOTA | 371 | CA | LEU | 155 | -17.829 | -8.353 | 9.204 | 1.00 20.04 |
| MOTA | 372 | CB | LEU | 155 | -17.524 | -8.428 | 7.692 | 1.00 20.81 |
| MOTA | 373 | CG | LEU | 155 | | -7.159 | 6.908 | 1.00 17.03 |
| ATOM | 374 | CD1 | LEU | 155 | -17.822 | | 7.139 | 1.00 12.42 |
| ATOM | 375 | CD2 | LEU | 155 | -17.912 | -9.810 | | 1.00 20.71 |
| ATOM | 376 | С | LEU | 155 | -20.055 | -7.187 | 9.904 | |
| ATOM | 377 | 0 | LEU | 155 | -20.712 | -8.163 | 10.217 | |
| ATOM | 378 | N | GLU | 15€ | -20.593 | -5.995 | 9.561 | 1.00 19.51 |
| ATOM | 379 | Н | GLU | 156 | -19.959 | -5.230 | 9.440 | 1.00 15.00 |
| ATOM | 380 | CA | GLU | 156 | -22.036 | -5.888 | 9.413 | 1.00 21.95 |
| ATOM | 381 | CB | GLU | 156 | -22.641 | -4.631 | 10.033 | 1.00 18.95 |
| ATOM | 382 | CG | GLU | 156 | -22.098 | -4.412 | 11.436 | 1.00 27.68 |
| MCTA | 383 | CD | GLU | 156 | -22.721 | -5.194 | 12.587 | 1.00 31.62 |
| ATOM | 384 | OE1 | GLU | 156 | -23.347 | -6.248 | 12.367 | 1.00 33.40 |
| ATOM | 385 | OE2 | GLU | 156 | -22.532 | -4.721 | 13.724 | 1.00 35.00 |
| ATOM | 386 | С | GLU | 156 | -22.457 | -5.966 | 7.964 | 1.00 25.36 |
| ATOM | 387 | 0 | GLU | 156 | -21.958 | -5.298 | 7.077 | 1.00 22.70 |
| ATOM | 388 | N | ASN | 157 | -23.437 | -6.808 | 7.696 | 1.00 30.92 |
| ATOM | 389 | Н | ASN | 157 | -23.594 | -7.590 | 8.300 | 1.00 15.00 |
| ATOM | 390 | CA | ASN | 157 | -23.804 | -6.620 | 6.300 | 1.00 33.31 |
| MOTA | 391 | CB | ASN | 157 | -23.856 | -7.970 | 5.614 | 1.00 31.69 |
| ATOM | 392 | CG | ASN | 157 | -23.669 | -7.693 | 4.168 | 1.00 27.70 |
| ATOM | 393 | CD1 | | 157 | -23.397 | -6.593 | 3.810 | 1.00 25.89 |
| ATOM | 394 | ND2 | | 157 | -23.893 | -8.640 | 3.275 | 1.00 41.69 |
| | 395 | HD21 | ASN | 157 | -24.069 | -9.603 | 3.467 | 1.00 15.00. |
| ATOM | 396 | HD22 | ASN | 157 | -23.745 | -8.295 | 2.340 | 1.00 15.00 |
| ATOM | 397 | C | ASN | 157 | -24.988 | -5.658 | 6.118 | 1.00 35.08 |
| ATOM | 398 | 0 | ASN | 157 | -26.107 | -5.949 | 6.499 | 1.00 37.06 |
| ATOM | | Ŋ | GLY | 158 | -24.746 | -4.443 | 5.560 | 1.00 40.03 |
| ATOM | 399 | H | GLY | 158 | -25.601 | -3.952 | 5.429 | 1.00 15.00 |
| ATOM | 400 | CA | GLY | 158 | -23.422 | -3.887 | 5.121 | 1.00 38.11 |
| ATOM | 401 | | GLY | 158 | -23.062 | -3.720 | 3.617 | 1.00 37.48 |
| ATOM | 402 | C O | GLY | 158 | -23.890 | -3.108 | 2.950 | 1.00 41.11 |
| MOTA | 403 | | | 159 | -21.867 | -4.220 | 3.135 | 1.00 32.75 |
| ATOM | 404 | N | LYS | 159 | -21.904 | -4.134 | 2.130 | 1.00 15.00 |
| ATOM | 405 | H | LYS | 159 | -20.828 | -4.928 | 3.962 | 1.00 27.83 |
| ATOM | 406 | CA | LYS | | -20.317 | -6.122 | 3.217 | 1.00 28.17 |
| MOTA | 407 | CB | LYS | 159 | -19.734 | -7.168 | 4.069 | 1.00 20.48 |
| MOTA | 408 | CG | LYS | 159 | -20.533 | -8.426 | 4.192 | 1.00 29.61 |
| ATOM | 409 | CD | LYS | 159 | -20.533 | -9.191 | 2.869 | 1.00 40.41 |
| MOTA | 410 | CE | LYS | 159 | | -10.663 | 2.986 | 1.00 40.88 |
| MOTA | 411 | NZ | LYS | 159 | | -11.087 | 2.035 | 1.00 15.00 |
| ATOM | 412 | HZI | | 159 | -20.739 -20.070 | -11.087 | 3.600 | 1.00 15.00 |
| MCTA | 413 | HZZ | | 159 | | -10.848 | 3.389 | 1.00 15.00 |
| ATOM | 414 | HZ3 | LYS | 159 | -21.738 | -4.065 | 4.463 | 1.00 26.08 |
| MCTA | 415 | Ξ. | LYS | 159 | -19.688 | | 3.696 | 1.00 28.01 |
| ATOM | 416 417 | \supset | LYS | 159 | -19.023 | -3.369 | 5.807 | 1.00 18.90 |
| ATOM | 417 | N | SLN | 160 | -19.683 | -3.990 | 6.319 | 1.00 15.00 |
| ATOM | 418 | Η | GLN | 150 | -20.211 | -4.674 | 6.464 | 1.00 13.89 |
| ATCM | 419 | CA | 31.X | 160 | -18.922 | -2.929 | 0.404 | 1.00 13.09 |
| | | | | | | | | |

FIGURE 17H

| | | | _ | | | | |
|------|------------|----------|-----|---------|--------|--------|------------|
| ATOM | 420 | CB GLN | 160 | -19.778 | -1.694 | 6.611 | 1.00 16.79 |
| ATOM | 421 | CG GLN | 150 | -20.881 | -1.896 | 7.633 | 1.00 18.34 |
| MOTA | 422 | CD GLN | 160 | -22.133 | -1.166 | 7.193 | 1.00 23.97 |
| ATOM | 423 | OE1 GLN | 160 | -23.088 | -0.970 | 7.893 | 1.30 31.18 |
| ATOM | 424 | NE2 GLN | 160 | -22.257 | -0.771 | 5.948 | 1.00 28.16 |
| ATOM | | HE21 GLN | 160 | -23.194 | -0.420 | 5.928 | 1.00 15.00 |
| MOTA | | HE22 GLN | 160 | -21.624 | -0.780 | 5.186 | 1.00 15.00 |
| ATOM | 427 | C GLN | 160 | -18.313 | -3.309 | 7.777 | 1.00 12.87 |
| ATOM | 428 | O GLN | 160 | -18.838 | -4.151 | 8.498 | 1.00 14.78 |
| | 429 | N LEU | 161 | -17.187 | -2.637 | 8.085 | 1.00 11.22 |
| ATOM | 430 | H LEU | 161 | -16.767 | -2.124 | 7.340 | 1.00 15.00 |
| ATOM | | CA LEU | 161 | -16.583 | -2.870 | 9.405 | 1.00 9.71 |
| ATOM | 431 | CB LEU | 161 | -15.052 | -2.939 | 9.390 | 1.00 4.67 |
| ATOM | 432 433 | CG LEU | 161 | -14.438 | -4.060 | 8.559 | 1.00 7.30 |
| ATOM | | CD1 LEU | 161 | -14.511 | -5.447 | 9.207 | 1.00 10.80 |
| MOTA | 434 | CD1 LEU | 161 | -12.964 | -3.794 | 8.389 | 1.00 5.48 |
| ATOM | 435 | | 161 | -17.082 | -1.836 | 10.412 | 1.00 10.17 |
| MOTA | 436 | C LEU | 161 | -16.826 | -0.657 | 10.341 | 1.00 13.36 |
| ATOM | 437 | O LEU | 162 | -17.848 | -2.338 | 11.375 | 1.00 16.94 |
| MOTA | 438 | N THR | 162 | -18.153 | -3.279 | 11.251 | 1.00 15.00 |
| MOTA | 439 | H THR | | -18.317 | -1.480 | 12.493 | 1.00 16.14 |
| ATOM | 440 | CA THR | 162 | -19.807 | -1.769 | 12.640 | 1.00 13.33 |
| MOTA | 441 | CB THR | 162 | -20.339 | -1.707 | 11.308 | 1.00 16.73 |
| MOTA | 442 | OG1 THR | 162 | -21.211 | -1.254 | 11.343 | 1.00 15.00 |
| ATOM | 443 | HG1 THR | 162 | -20.553 | -0.832 | 13.562 | 1.00 15.01 |
| ATOM | 444 | CG2 THR | 162 | -20.553 | -1.547 | 13.842 | 1.00 13.28 |
| MOTA | 445 | C THR | 162 | -17.358 | -2.587 | 14.449 | 1.00 20.21 |
| MOTA | 446 | O THR | 162 | -16.994 | -0.437 | 14.282 | 1.00 14.22 |
| MOTA | 447 | N VAL | 163 | -16.859 | 0.243 | 13.567 | 1.00 15.00 |
| ATOM | 448 | H VAL | 163 | | -0.358 | 15.586 | 1.00 15.72 |
| ATOM | 449 | CA VAL | 163 | -16.326 | 0.426 | 15.428 | 1.00 11.82 |
| MOTA | 450 | CB VAL | 163 | -15.038 | 1.944 | 15.368 | 1.00 9.87 |
| ATOM | 451 | CG1 VAL | 163 | -15.191 | -0.124 | 14.245 | 1.00 18.88 |
| ATOM | 452 | CG2 VAL | 163 | -14.229 | 0.283 | 16.706 | 1.00 17.93 |
| ATOM | 453 | C VAL | 163 | -17.193 | | 16.453 | 1.00 20.25 |
| MOTA | 454 | O VAL | 163 | -18.001 | 1.180 | 17.925 | 1.00 15.44 |
| ATOM | 455 | N LYS | 164 | -17.037 | -0.232 | 18.020 | 1.00 15.00 |
| ATOM | 456 | H LYS | 164 | -16.254 | -0.858 | 19.109 | 1.00 17.33 |
| ATOM | 457 | CA LYS | 164 | -17.856 | 0.138 | 19.807 | 1.00 19.58 |
| MOTA | 458 | CB LYS | | -18.351 | -1.150 | 18.759 | 1.00 23.56 |
| ATOM | 459 | CG LYS | 164 | -19.214 | -1.885 | 18.851 | 1.00 28.85 |
| ATOM | 460 | CD LYS | | -19.417 | -3.410 | 17.554 | 1.00 23.81 |
| ATOM | 461 | CE LYS | | -20.039 | -4.047 | | 1.00 18.98 |
| MOTA | 462 | NZ LYS | | -19.428 | -3.681 | 16.227 | 1.00 15.00 |
| ATOM | 463 | HZ1 LYS | | -19.195 | -2.667 | 16.222 | 1.00 15.00 |
| ATOM | 464 | HZ2 LYS | | -18.552 | -4.223 | 16.092 | 1.00 15.00 |
| ATOM | 465 | HZ3 IYS | | -20.084 | -3.888 | 15.445 | 1.00 15.14 |
| MOTA | 466 | C LYS | | -17.193 | 1.099 | 20.056 | 1.00 13.14 |
| ATOM | 467 | O LYS | | -17.712 | 1.588 | 21.048 | 1.00 17.72 |
| ATOM | 468 | n Arc | | -15.992 | 1.428 | 19.621 | 1.00 17.49 |
| ATOM | 469 | H ARC | | -15.550 | 0.838 | 18.932 | 1.00 20.18 |
| ATOM | 470 | CA ARC | | -15.184 | 2.415 | 20.325 | |
| MOTA | 471 | CB ARC | | -13.985 | 1.806 | 21.049 | 1.00 24.65 |
| MCTA | 472 | CG ARC | | -14.363 | 0.833 | 22.126 | 1.00 29.54 |
| ATOM | 473 | CD ARC | | -13.274 | 1.077 | 23.145 | 1.00 38.82 |
| MOTA | 474 | NE ARC | | -13.719 | 1.998 | 24.186 | 1.00 43.41 |
| MCTA | 475 | HE AR | 165 | -14.331 | 1.671 | 24.908 | 1.00 15.00 |
| ATOM | 475 | CZ AR | 165 | -13.190 | 3.250 | 24.362 | 1.00 44.06 |
| MCTA | 477 | NH1 AR | 165 | -13.406 | 3.765 | 25.562 | 1.00 41.25 |
| MCTA | 478 | | | -13.054 | 4.683 | 25.763 | 1.00 15.00 |
| ATOM | 479 | | | -13.919 | 3.249 | 26.250 | 1.00 15.00 |
| | | | | | | | |

FIGURE 17I

| ATOM | 480 | NH2 | ARG | 165 | -12.485 | 3.946 | 23.425 | 1.00 31.65 | A |
|------|-----|------------|-----|-----|---------|--------|--------|------------|------------|
| ATOM | 481 | HH21 | ARG | 165 | -12.133 | 4.860 | 23.623 | 1.00 15.00 | A |
| MOTA | 482 | HH22 | ARG | 165 | -12.322 | 3.527 | 22.530 | 1.00 15.00 | A |
| ATOM | 483 | \subset | ARG | 165 | -14.608 | 3.554 | 19.510 | 1.00 17.70 | À |
| MOTA | 484 | 0 | ARG | 165 | -14.018 | 3.450 | 18.441 | 1.00 18.26 | A |
| ATOM | 485 | N | GLN | 166 | -14.763 | 4.687 | 20.151 | 1.00 17.43 | A |
| ATOM | 486 | Н | GLN | 166 | -15.263 | 4.614 | 21.007 | 1.00 15.00 | . A |
| ATOM | 487 | CA | GLN | 166 | -14.138 | 5.911 | 19.698 | 1.00 19.00 | A |
| ATOM | 488 | CB | GLN | 166 | -14.613 | 7.021 | 20.610 | 1.00 23.79 | A |
| ATOM | 489 | CG | GLN | 166 | -14.067 | 8.409 | 20.386 | 1.00 34.06 | A |
| ATOM | 490 | CD | GLN | 166 | -15.178 | 9.399 | 20.659 | 1.00 45.91 | A |
| ATOM | 491 | OE1 | GLN | 166 | -15.102 | 10.492 | 20.135 | 1.00 53.64 | Α |
| ATOM | 492 | NE2 | GLN | 166 | -16.202 | 9.046 | 21.418 | 1.00 44.10 | A |
| ATOM | 493 | HE21 | GLN | 166 | -16.906 | 9.765 | 21.443 | 1.00 15.00 | Α |
| ATOM | 494 | HE22 | GLN | 166 | -16.577 | 8.287 | 21.935 | 1.00 15.00 | Α |
| ATOM | 495 | C | GLN | 166 | -12.649 | 5.881 | 19.644 | 1.00 17.48 | A |
| ATOM | 496 | 0 | GLN | 166 | -12.029 | 5.378 | 20.561 | 1.00 18.13 | A |
| ATOM | 497 | N | GLY | 167 | -12.160 | 6.478 | 18.565 | 1.00 14.83 | Α |
| ATOM | 498 | H | GLY | 167 | -12.750 | 6.836 | 17.850 | 1.00 15.00 | A |
| ATOM | 499 | CA | GLY | 167 | -10.728 | 6.711 | 18.557 | 1.00 16.28 | A |
| ATOM | 500 | C | GLY | 167 | -10.044 | 6.685 | 17.204 | 1.00 16.48 | A |
| MOTA | 501 | 0 | GLY | 167 | -10.674 | 6.601 | 16.162 | 1.00 19.19 | A |
| ATOM | 502 | N | LEU | 168 | -8.720 | 6.735 | 17.209 | 1.00 17.06 | . A |
| ATOM | 503 | Н | LEU | 168 | -8.311 | 6.890 | 18.120 | 1.00 15.00 | A |
| MOTA | 504 | CA | LEU | 168 | -7.925 | 6.625 | 15.992 | 1.00 16.60 | Α |
| ATOM | 505 | CB | LEU | 168 | -6.600 | 7.343 | 16.289 | 1.00 21.87 | A |
| ATOM | 506 | CG | LEU | 168 | -6.247 | 8.745 | 15.716 | 1.00 22.69 | A |
| ATOM | 507 | CD1 | LEU | 168 | -5.119 | 9.410 | 16.539 | 1.00 21.20 | А |
| ATOM | 508 | | LEU | 168 | -7.436 | 9.617 | 15.361 | 1.00 18.38 | A |
| ATOM | 509 | C | LEU | 168 | -7.686 | 5.136 | 15.604 | 1.00 14.84 | A |
| ATOM | 510 | 0 | LEU | 168 | -7.282 | 4.278 | 16.392 | 1.00 15.89 | A |
| ATOM | 511 | N | TYR | 169 | -7.943 | 4.873 | 14.300 | 1.00 10.57 | A |
| ATOM | 512 | H | TYR | 169 | -8.313 | 5.659 | 13.807 | 1.00 15.00 | A |
| ATOM | 513 | CA | TYR | 169 | -7.683 | 3.572 | 13.656 | 1.00 5.27 | A |
| ATOM | 514 | CB | TYR | 169 | -8.989 | 3.014 | 13.230 | 1.00 5.83 | A |
| ATOM | 515 | CG | TYR | 169 | -9.857 | 2.620 | 14.423 | 1.00 6.94 | A |
| MOTA | 516 | CD1 | TYR | 169 | -10.524 | 3.598 | 15.168 | 1.00 7.40 | A |
| ATOM | 517 | CE1 | TYR | 169 | -11.390 | 3.193 | 16.218 | 1.00 7.77 | A |
| ATOM | 518 | CD2 | TYR | 169 | -10.016 | 1.255 | 14.744 | 1.00 8.89 | A |
| ATOM | 519 | CE2 | TYR | 169 | -10.850 | 0.841 | 15.804 | 1.00 9.40 | A |
| ATOM | 520 | CZ | TYR | 169 | -11.563 | 1.827 | 16.534 | 1.00 10.39 | A |
| ATOM | 521 | ОН | TYR | 169 | -12.443 | 1.410 | 17.534 | 1.00 7.99 | Ā |
| ATOM | 522 | нн | TYR | 169 | -13.009 | 2.117 | 17.800 | 1.00 15.00 | A |
| ATOM | 523 | C | TYR | 169 | -6.810 | 3.642 | 12.390 | 1.00 6.72 | A |
| MOTA | 524 | 0 | TYR | 169 | -6.917 | 4.498 | 11.557 | 1.00 9.12 | A |
| ATOM | 525 | N | TYR | 170 | -5.899 | 2.722 | 12.228 | 1.00 9.53 | A |
| ATOM | 526 | H | TYR | 170 | -5.806 | 2.081 | 12.986 | 1.00 15.00 | A |
| ATOM | 527 | CA | TYR | 170 | -5.313 | 2.511 | 10.899 | 1.00 10.01 | A |
| ATOM | 528 | CB | TYR | 170 | -3.967 | 1.797 | 11.044 | 1.00 7.46 | A |
| MOTA | 529 | CG | TYR | 170 | -3.259 | 1.636 | 9.679 | 1.00 13.45 | A |
| ATOM | 530 | CD1 | TYR | 170 | -2.680 | 2.766 | 9.052 | 1.00 12.66 | A |
| ATOM | 531 | CE1 | TYR | 170 | -2.213 | 2.658 | 7.738 | 1.00 10.18 | A |
| ATOM | 532 | CD2 | TYR | 170 | -3.304 | 0.385 | 9.057 | 1.00 10.90 | A |
| ATOM | 533 | CE2 | TYR | 170 | -2.891 | 0.303 | 7.730 | 1.00 8.68 | A |
| MOTA | 534 | CZ | TYR | 170 | -2.331 | 1.419 | 7.124 | 1.00 9.97 | A |
| MOTA | 535 | OH | TYR | 170 | -1.774 | 1.286 | 5.859 | 1.00 17.50 | A |
| ATOM | 536 | нн | TYR | 170 | -1.886 | 0.404 | 5.514 | 1.00 15.00 | A |
| ATOM | 537 | C . | TYR | 170 | -6.279 | 1.610 | 10.073 | 1.00 10.40 | A |
| ATOM | 538 | 0 | TYR | 170 | -6.679 | 0.500 | 10.421 | 1.00 12.52 | A |
| ATOM | 539 | N | ILE | 171 | -6.704 | 2.174 | 8.968 | 1.00 12.16 | A |

FIGURE 17J

| | 540 | H | ILE | 171 | -5.475 | 3.135 | 8.808 | 1.00 15.00 |
|------|-------|------|-----|-----|---------|--------|---------|------------|
| MCTA | | | ILE | 171 | -7.608 | 1.430 | 8.138 | 1.00 9.37 |
| ATOM | 541 | CA | | 171 | -9.070 | 1.990 | 8.317 | 1.00 11.21 |
| MOTA | 542 | CB | ILE | | -9.326 | 3.501 | 8.677 | 1.00 17.27 |
| MOTA | 543 | CG2 | ILE | 171 | | | | 1.00 13.33 |
| ATOM | 544 | CG1 | ILE | 171 | -10.046 | 1.564 | 7.214 | |
| MOTA | 545 | CD1 | ILE | 171 | -10.647 | 0.250 | 7.619 | 1.00 17.53 |
| ATOM | 546 | С | ILE | 171 | -7.074 | 1.234 | 6.694 | 1.00 8.34 |
| ATOM | 547 | 0 | ILE | 171 | -6.453 | 2.088 | 6.082 | 1.00 6.96 |
| ATOM | 548 | N | TYR | 172 | -7.286 | 0.005 | 6.216 | 1.00 11.07 |
| ATOM | 549 | H | TYR | 172 | -7.809 | -0.624 | 6.786 | 1.00 15.00 |
| | 550 | CA | TYR | 172 | -6.708 | -0.378 | 4.922 | 1.00 15.60 |
| ATOM | | CB | TYR | 172 | -5.332 | -1.082 | 5.037 | 1.00 14.32 |
| MOTA | 551 | | TYR | 172 | -5.389 | -2.397 | 5.796 | 1.00 9.21 |
| ATOM | 552 | CG | | | -5.342 | -2.402 | 7.216 | 1.00 12.52 |
| ATOM | 553 | CD1 | TYR | 172 | -5.607 | -3.620 | 7.901 | 1.00 10.88 |
| ATOM | 554 | CEl | TYR | 172 | | -3.586 | 5.050 | 1.00 12.66 |
| ATOM | 555 | CD2 | TYR | 172 | -5.565 | | | |
| ATOM | 556 | CE2 | TYR | 172 | -5.829 | -4.800 | 5.740 | 1.00 15.83 |
| ATOM | 557 | CZ | TYR | 172 | -5.822 | -4.808 | 7.164 | 1.00 11.94 |
| ATOM | 558 | OH | TYR | 172 | -5.995 | -6.002 | 7.820 | 1.00 12.17 |
| ATOM | 559 | нн | TYR | 172 | -6.433 | -5.843 | 8.657 | 1.00 15.00 |
| ATOM | 560 | C | TYR | 172 | -7.605 | -1.276 | 4.106 | 1.00 16.85 |
| | 561 | Õ | TYR | 172 | -8.346 | -2.057 | 4.692 | 1.00 14.06 |
| MOTA | | й | ALA | 173 | -7.448 | -1.141 | 2.776 | 1.00 16.29 |
| MCTA | 562 | | ALA | 173 | -6.751 | -0.490 | 2.503 | 1.00 15.00 |
| ATOM | 563 | H | | | -7.940 | -2.152 | 1.836 | 1.00 15.11 |
| ATOM | 564 | CA | ALA | 173 | | | 1.292 | 1.00 12.08 |
| ATOM | 565 | CB | ALA | 173 | -9.300 | -1.725 | | |
| MOTA | 566 | C | ALA | 173 | -7.007 | -2.537 | 0.653 | 1.00 15.86 |
| ATOM | 567 | 0 | ALA | 173 | -6.147 | -1.806 | 0.191 | 1.00 14.20 |
| MOTA | 568 | N | GLN | 174 | -7.244 | -3.714 | 0.109 | 1.00 16.56 |
| ATOM | 569 | Н | GLN | 174 | -7.774 | -4.389 | 0.620 | 1.00 15.00 |
| ATOM | 570 | CA | GLN | 174 | -6.470 | -4.119 | -1.070 | 1.00 19.25 |
| ATOM | 571 | CB | GLN | 174 | -5.582 | -5.292 | -0.832 | 1.00 21.99 |
| | 572 | CG | GLN | 174 | -4.205 | -4.727 | -1.030 | 1.00 30.99 |
| ATOM | 573 | CD | GLN | 174 | -3.174 | -5.845 | -0.979 | 1.00 34.25 |
| ATOM | | | GLN | 174 | -2.308 | -5.899 | -0.105 | 1.00 32.91 |
| ATOM | 574 | OE1 | | | -3.268 | -6.699 | -2.014 | 1.00 31.50 |
| ATOM | 575 | | GLN | 174 | -2.668 | -7.487 | -1.970 | 1.00 15.00 |
| MOTA | 576 | HE21 | | 174 | | | -2.714 | 1.00 15.00 |
| MOTA | 577 | HE22 | | 174 | -3.973 | -6.621 | | 1.00 19.20 |
| ATOM | 578 | C | GLN | 174 | -7.413 | -4.644 | -2.114 | _ |
| ATOM | 579 | 0 | GLN | 174 | -8.285 | -5.434 | -1.880 | 1.00 20.03 |
| ATOM | 580 | N | VAL | 175 | -7.291 | -4.107 | -3.301 | 1.00 19.28 |
| ATOM | 581 | н | VAL | 175 | -6.594 | -3.401 | -3.400 | 1.00 15.00 |
| MCTA | 582 | CA | VAL | 175 | -8.247 | -4.500 | -4.323 | 1.00 22.43 |
| ATOM | 583 | CB | VAL | 175 | -9.319 | -3.409 | -4.644 | 1.00 21.41 |
| ATOM | 584 | CG1 | | 175 | -10.146 | -2.830 | -3.495 | 1.00 20.17 |
| | | | VAL | 175 | -10.268 | -4.061 | -5.639 | 1.00 22.88 |
| MOTA | 585 | | | 175 | -7.508 | -4.859 | -5.615 | 1.00 24.56 |
| ATOM | 586 | C | VAL | | -6.928 | -3.997 | -6.301 | 1.00 23.28 |
| MCTA | 587 | 0 | VAL | 175 | | | -5.879 | 1.00 25.40 |
| MOTA | 588 | N | THR | 176 | -7.563 | -6.180 | -5.250 | 1.00 15.00 |
| ATOM | 589 | Н | THR | 176 | -7.994 | -6.850 | | |
| ATOM | 590 | CA | THR | 176 | -7.086 | -6.501 | -7.222 | 1.00 24.46 |
| MCTA | 591 | CB | THR | 176 | -5.844 | -7.454 | -7.256 | 1.00 24.78 |
| MCTA | . 592 | OG: | | 176 | -5.948 | -8.650 | -8.028 | 1.00 20.31 |
| MCTA | 593 | HG1 | | 176 | -5.250 | -9.253 | -7.796 | 1.00 15.00 |
| ATOM | 594 | CG2 | | 76 | -5.329 | -7.711 | -5.867 | 1.00 17.07 |
| ATOM | 595 | 5 | THR | :76 | -8.178 | -6.700 | -8.272 | 1.00 25.44 |
| | | | THR | 176 | -9.326 | -7.043 | -7.995 | 1.00 26.86 |
| ATOM | 596 | | | 177 | -7.855 | -6.341 | -9.506 | 1.00 22.44 |
| ATOM | 597 | | PHE | | -6.920 | -6.083 | -9.732 | 1.00 15.00 |
| ATOM | 598 | | PHE | 177 | -8.939 | | -10.479 | 1.00 22.70 |
| ATOM | 599 | CA | PHE | 177 | -0.737 | J.J.1 | | |
| | | | | | | | | |

FIGURE 17K

| FIGURE 17K | | | | | | | | | | |
|--|---|--|---|--|--|--|--|--|--|--|
| ATOM ATOM ATOM ATOM ATOM ATOM | 600 CB 601 CG 602 CD1 603 CD2 604 CE1 605 CE2 606 CZ | PHE PHE | 177 177 177 177 177 177 | -9.746 -8.813 -8.771 -8.011 -8.041 -7.289 | -5.194 -10.599 -4.034 -10.927 -3.548 -12.252 -3.422 -9.920 -2.387 -12.550 -2.247 -10.204 -1.713 -11.500 | 1.00 20.90 1.00 22.51 1.00 22.11 1.00 21.87 1.00 20.53 1.00 20.44 1.00 22.79 | | | | |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 607 C 608 O 609 N 610 H 611 CA 612 CB 613 SG 614 C | PHE PHE CYS CYS CYS CYS CYS | 177 177 178 178 178 178 178 | -8.381 -7.219 -9.210 -10.146 -8.599 -8.501 -7.685 -9.323 | -6.949 -11.800 -6.695 -12.072 -7.555 -12.625 -7.797 -12.370 -7.849 -13.942 -9.365 -14.214 -9.731 -15.792 -7.146 -15.088 | 1.00 22.14 1.00 21.60 1.00 24.52 1.00 15.00 1.00 29.77 1.00 32.06 1.00 35.17 1.00 28.41 | | | | |
| ATOM ATOM ATOM ATOM ATOM ATOM | 615 O 616 N 617 H 618 CA 619 CB 620 OG 621 HG | CYS SER SER SER SER SER SER SER | 178 179 179 179 179 179 179 | -10.534 -8.589 -7.608 -9.374 -9.379 -10.615 -10.725 -9.063 | -7.247 -15.185 -6.393 -15.910 -6.271 -15.754 -5.454 -16.704 -4.118 -16.020 -3.492 -16.319 -2.812 -15.667 -5.196 -18.165 | 1.00 27.54 1.00 28.86 1.00 15.00 1.00 29.01 1.00 30.82 1.00 39.79 1.00 15.00 1.00 31.16 | | | | |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 622 C 623 O 624 N 625 H 626 CA 627 CB 628 CG 629 ODI | SER ASN ASN ASN ASN ASN | 179 180 180 180 180 180 180 | -7.931 -10.083 -10.966 -9.782 -10.205 -9.650 -10.058 -8.619 | -4.953 -18.537 -5.255 -19.042 -5.700 -18.834 -4.725 -20.366 -5.554 -21.589 -4.980 -22.896 -3.947 -23.356 -5.536 -23.456 | 1.00 28.58 1.00 35.32 1.00 15.00 1.00 34.74 1.00 37.96 1.00 37.12 1.00 40.66 1.00 35.85 | | | | |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 630 ND2 631 HD21 632 HD22 633 C 634 O 635 N 636 H | ASN | 180 180 180 180 181 181 181 | -8.343 -8.153 -10.197 -11.314 -9.147 -6.363 -8.997 -7.563 | -6.475 -23.306 -4.891 -24.065 -3.331 -20.588 -2.894 -20.433 -2.699 -21.068 -3.318 -21.141 -1.313 -21.489 -1.279 -22.026 | 1.00 15.00 1.00 15.00 1.00 36.96 1.00 37.89 1.00 41.95 1.00 15.00 1.00 44.24 1.00 43.43 | | | | |
| ATOM ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 645 HH1 | ARG ARG ARG ARG ARG 1 ARG | 181 181 181 181 181 181 | -6.348 -6.235 -5.064 -4.991 -4.024 -2.886 -2.113 -2.807 | -1.638 -21.101 -2.853 -20.134 -2.772 -19.271 -2.058 -18.578 -3.611 -19.432 -3.414 -18.790 -4.032 -18.918 -2.642 -18.161 | 1.00 45.11 1.00 40.68 1.00 46.11 1.00 15.00 1.00 49.77 1.00 54.33 1.00 15.00 | | | | |
| MOTA ATOM ATOM ATOM ATOM ATOM ATOM ATOM | 648 HH2 649 HH2 650 C 651 O 652 N 653 H | 2 ARG 1 ARG 2 ARG ARG ARG GLU GLU | 181 181 181 181 181 191 182 | -4.085 -3.286 -4.918 -10.049 -10.979 -9.895 -9.201 | -4.641 -20.247 -5.230 -20.354 -4.833 -20.761 -0.866 -22.499 -0.112 -22.227 -1.447 -23.690 -2.166 -23.775 | 1.00 54.26 1.00 15.00 1.00 15.00 1.00 47.10 1.00 49.20 1.00 49.64 1.00 15.00 1.00 52.41 | | | | |
| ATOM ATOM ATOM ATOM ATOM ATOM | 554 CA 655 CB 656 CG 657 CD 658 OE 659 OE | GLU GLU GLU | 182 182 182 182 182 182 | -10.976 -10.437 -10.932 -10.758 -9.613 -11.778 | -1.385 -24.676 -2.020 -25.970 -1.418 -27.295 0.116 -27.327 0.586 -27.442 0.830 -27.244 | 1.00 56.93 1.00 66.05 1.00 70.54 1.00 72.98 1.00 72.46 | | | | |

FIGURE 17L

| ATOM | 660 | C | GLU | 182 | -12.388 | -7 934 | -24.304 | 1.00 53.00 |
|------|-----|------|-----|-----|---------|--------|--------------------|------------|
| ATOM | 661 | Ö | GLU | 182 | -13.379 | | -24.862 | 1.00 54.27 |
| MCTA | 662 | N | ALA | 183 | -12.505 | | -23.335 | 1.00 52.34 |
| MCTA | 663 | Н | ALA | 183 | -11.676 | | -22.865 | 1.00 15.00 |
| ATOM | 664 | CA | ALA | 183 | -13.867 | | -22.899 | 1.00 50.19 |
| ATOM | 665 | CB | ALA | 183 | -13.855 | | -22.447 | 1.00 45.02 |
| ATOM | 666 | C | ALA | 183 | -14.562 | | -21.867 | 1.00 45.02 |
| ATOM | 667 | 0 | ALA | 183 | -15.712 | | -21.990 | |
| ATOM | 668 | N | SER | 184 | -13.773 | | | 1.00 47.77 |
| ATOM | 669 | H | SER | 184 | -12.826 | | -20.878 -20.991 | 1.00 52.95 |
| ATOM | 670 | CA | SER | 184 | -14.228 | | -19.729 | 1.00 15.00 |
| ATOM | 671 | CB | SER | 184 | -13.384 | | | 1.00 56.78 |
| | 672 | OG | SER | 184 | -13.364 | | -18.481 | 1.00 53.58 |
| ATOM | 673 | НG | SER | | | | -17.721 | 1.00 47.46 |
| ATOM | | | | 184 | -13.291 | | -17.388 | 1.00 15.00 |
| MOTA | 674 | C | SER | 184 | -14.183 | | -19.880 | 1.00 59.95 |
| ATOM | 675 | 0 | SER | 184 | -13.913 | | -18.964 | 1.00 65.25 |
| ATOM | 676 | N | SER | 185 | -14.324 | | -21.131 | 1.00 60.08 |
| ATOM | 677 | H | SER | 185 | -14.623 | | -21.831 | 1.00 15.00 |
| ATOM | 678 | CA | SER | 185 | -13.825 | | -21.391 | 1.00 60.12 |
| ATOM | 679 | CB | SER | 185 | -13.522 | 2.640 | -22.869 | 1.00 60.49 |
| ATOM | 680 | OG | SER | 185 | -12.243 | | -23.242 | 1.00 59.80 |
| ATOM | 681 | HG | SER | 185 | -12.158 | 1.234 | -22.833 | 1.00 15.00 |
| ATOM | 682 | C | SER | 185 | -14.580 | | -20.885 | 1.00 59.59 |
| ATOM | 683 | 0 | SER | 185 | -15.437 | | -21.543 | 1.00 60.08 |
| ATOM | 684 | N | GLN | 186 | -14.200 | | | 1.00 57.71 |
| ATOM | 685 | H | GLN | 186 | -13.601 | | -19.153 | 1.00 15.00 |
| ATOM | 686 | CA | GLN | 186 | -15.121 | | -18.993 | 1.00 57.00 |
| ATOM | 687 | CB | GLN | 186 | -16.094 | | -18.175 | 1.00 58.66 |
| ATOM | 688 | CG | GLN | 186 | -15.355 | | -17.050 | 1.00 59.69 |
| ATOM | 689 | CD | GLN | 186 | -16.369 | | -16.088 | 1.00 59.92 |
| MCTA | 690 | | GLN | 186 | -17.270 | | | 1.00 59.81 |
| ATOM | 691 | NE2 | | 186 | -16.249 | | -15.787 | 1.00 59.63 |
| ATOM | | HE21 | | 186 | -15.492 | | -16.113 | 1.00 15.00 |
| ATOM | | | GLN | 186 | -16.950 | | -15.168 | 1.00 15.00 |
| ATOM | 694 | C | GLN | 186 | -14.758 | | -18.221 | 1.00 54.36 |
| ATOM | 695 | 0 | GLN | 186 | -15.596 | | -18.298 | 1.00 53.98 |
| ATOM | 696 | N | ALA | 187 | -13.566 | | -17.511 | 1.00 50.35 |
| ATOM | 697 | H | ALA | 187 | -13.476 | | -16.970 | 1.00 15.00 |
| MOTA | 698 | CA | ALA | 187 | -12.388 | | -17.832 | 1.00 43.26 |
| ATOM | 699 | CB | ALA | 187 | -11.546 | | -18.918 | 1.00 38.95 |
| MCTA | 700 | C | ALA | 187 | -11.456 | | -16.849 | 1.00 40.48 |
| MOTA | 701 | 0 | ALA | 187 | -10.887 | | -17.295 | 1.00 43.24 |
| MOTA | 702 | N | PRO | 188 | -11.210 | | -15.594 | 1.00 38.66 |
| ATOM | 703 | CD | PRO | 188 | -11.543 | | -15.000 | 1.00 38.15 |
| | 704 | CA | PRO | 188 | -10.220 | | -14.751 | |
| MOTA | 705 | CB | PRO | 188 | -9.395 | | -14.150 | 1.00 33.99 |
| ATOM | 706 | CG | PRO | 188 | -10.377 | | -14.036 | 1.00 32.69 |
| ATOM | 707 | Ç | PRO | 188 | -10.840 | | -13.683 | 1.00 33.66 |
| MOTA | 708 | 0 | PRO | 188 | -11.885 | | -13.140 | 1.00 33.41 |
| ATOM | 709 | N | PHE | 189 | -10.147 | | -13.346 | 1.00 28.66 |
| ATOM | 710 | Н | PHE | 189 | -9.260 | | -13.748 | 1.00 15.00 |
| MOTA | 711 | CA | PHE | 189 | -10.721 | | -12.171 | 1.00 26.71 |
| | 712 | CB | PHE | 189 | -10.122 | | -12.034 | 1.00 26.21 |
| ATOM | 713 | CG | PHE | 189 | -10.671 | | -10.849 | 1.00 22.92 |
| MOTA | 714 | CD1 | PHE | 189 | -10.126 | 0.005 | -9.566 | 1.00 17.72 |
| ATOM | 715 | CD2 | PHE | 199 | -11.687 | | -11.064 | 1.00 21.88 |
| MCTA | 716 | CEI | PHE | 189 | -10.590 | -0.815 | -8.522 | 1.00 19.12 |
| ATOM | 717 | CE2 | PHE | 189 | -12.124 | | -10.011 | 1.00 21.13 |
| ATOM | 718 | ςz | PHE | 189 | -11.571 | -1.806 | -8.736 | 1.00 18.44 |
| ATOM | 719 | C | PHE | 189 | -10.445 | 2.815 | -10.909 | 1.00 27.14 |
| | | | | | | | | |

34/46

FIGURE 17M

| | | | | | | | | • |
|--------------|-----|-----|----------------|------|------------|---------|---------|------------|
| | | _ | 21.2 | - 00 | -9.308 | 3 244 . | -10.706 | 1.00 28.72 |
| ATOM | 720 | 0 | PHE | .189 | | 2.244 | -10.071 | 1.00 24.71 |
| MCTA | 721 | N | ILE | 190 | -11.468 | | -10.389 | 1.00 15.00 |
| ATOM | 722 | H | ILE | 190 | -12.408 | _ | | 1.00 24.03 |
| ATOM | 723 | CA | ILE | 190 | -11.193 | 3.626 | -8.789 | 1.00 26.86 |
| MOTA | 724 | CB | ILE | 190 | -11.316 | 5.242 | -8.743 | |
| ATOM | 725 | CG2 | ILE | 190 | -11.892 | 5.979 | -9.997 | 1.00 19.87 |
| ATOM | 726 | CGl | ILE | 190 | -11.801 | 5.888 | -7.424 | 1.00 22.54 |
| ATOM | 727 | CD1 | ILE | 190 | -12.819 | 7.012 | -7.645 | 1.00 28.56 |
| ATOM | 728 | C | ILE | 190 | -11.844 | 2.812 | -7.656 | 1.00 21.97 |
| ATOM | 729 | 0 | ILE | 190 | -12.891 | 2.197 | -7.801 | 1.00 16.30 |
| ATOM | 730 | N | ALA | 191 | -11.026 | 2.700 | -6.590 | 1.00 17.21 |
| ATOM | 731 | Н | ALA | 191 | -10.124 | 3.124 | -6.662 | 1.00 15.00 |
| ATOM | 732 | CA | ALA | 191 | -11.501 | 2.195 | -5.321 | 1.00 15.20 |
| ATOM | 733 | CB | ALA | 191 | -10.730 | 0.928 | -4.968 | 1.00 14.79 |
| ATOM | 734 | c | ALA | 191 | -11.439 | 3.230 | -4.206 | 1.00 17.11 |
| ATOM | 735 | ō | ALA | 191 | -10.467 | 3.961 | -4.052 | 1.00 14.04 |
| | 736 | N | SER | 192 | -12.511 | 3.245 | -3.433 | 1.00 14.72 |
| ATOM ATOM | 737 | Н | SER | 192 | | 2.694 | -3.804 | 1.00 15.00 |
| | 738 | CA | SER | 192 | -12.725 | 4.289 | -2.423 | 1.00 16.69 |
| ATOM | 739 | CB | SER | 192 | -13.931 | 5.144 | -2.803 | 1.00 14.83 |
| ATOM | | | SER | 192 | -13.556 | 5.828 | -3.994 | 1.00 21.23 |
| ATOM | 740 | OG | | 192 | -14.367 | 5.966 | -4.520 | 1.00 15.00 |
| ATOM | 741 | HG | SER | | -12.980 | 3.682 | -1.069 | 1.00 17.77 |
| ATOM | 742 | C | SER | 192 | -13.753 | 2.738 | -0.947 | 1.00 20.76 |
| ATOM | 743 | 0 | SER | 192 | -12.285 | 4.209 | -0.038 | 1.00 15.56 |
| MOTA | 744 | N | LEU | 193 | | 4.259 | -0.280 | 1.00 15.00 |
| ATOM | 745 | H | LEU | 193 | -11.681 | | 1.366 | 1.00 13.27 |
| ATOM | 746 | CA | LEU | 193 | -12.510 | 3.761 | | 1.00 13.27 |
| MOTA | 747 | CB | LEU | 193 | -11.195 | 3.825 | 2.217 | 1.00 12.74 |
| ATOM | 748 | CG | LEU | 193 | -11.051 | 3.141 | 3.604 | 1.00 14.57 |
| MOTA | 749 | CD1 | | 193 | -12.272 | 2.354 | 4.116 | 1.00 14.67 |
| ATOM | 750 | | LEU | 193 | -10.274 | 3.986 | 4.622 | |
| ATOM | 751 | C | LEU | 193 | -13.497 | 4.748 | 1.911 | 1.00 11.22 |
| ATOM | 752 | 0 | LEU | 193 | -13.188 | 5.912 | 1.903 | 1.00 12.22 |
| ATOM | 753 | N | CYS | 194 | -14.652 | 4.326 | 2.310 | 1.00 13.66 |
| MOTA | 754 | H | CYS | 194 | -14.828 | 3.347 | 2.276 | 1.00 15.00 |
| ATOM | 755 | CA | CYS | 194 | -15.595 | 5.360 | 2.713 | 1.00 14.84 |
| ATOM | 756 | CB | CYS | 194 | -16.915 | 5.409 | 1.918 | 1.00 17.58 |
| ATOM | 757 | SG | CYS | 194 | -16.623 | 5.417 | 0.165 | 1.00 16.33 |
| ATOM | 758 | C | CYS | 194 | -16.046 | 5.163 | 4.137 | 1.00 12.81 |
| ATOM | 759 | 0 | CYS | 194 | -15.983 | 4.072 | 4.655 | 1.00 10.34 |
| ATOM | 760 | N | LEU | 195 | -16.557 | 6.254 | 4.697 | 1.00 14.32 |
| ATOM | 761 | Н | LEU | 195 | -16.541 | 7.088 | 4.154 | 1.00 15.00 |
| ATOM | 762 | CA | LEU | 195 | -17.039 | 6.291 | 6.076 | 1.00 14.89 |
| ATOM | 763 | CB | LEU | 195 | -16.195 | 7.372 | 6.789 | 1.00 15.56 |
| ATOM | 764 | CG | LEU | 195 | -16.571 | 7.680 | 8.242 | 1.00 15.56 |
| ATOM | 765 | 551 | LEU | 195 | -15.932 | 8.967 | 8.762 | 1.00 13.72 |
| MOTA | 765 | | LEU | 195 | -16.463 | 6.448 | 9.154 | 1.00 17.25 |
| ATOM | 767 | C | LEU | 195 | -18.546 | 6.544 | 6.209 | 1.00 13.54 |
| ATOM | 768 | 0 | LEU | 195 | -19.038 | 7.521 | 5.705 | 1.00 14.56 |
| ATOM | 769 | N | LYS | 196 | -19.238 | 5.667 | 6.905 | 1.00 16.36 |
| | 770 | H | LYS | 196 | -18.719 | 4.875 | 7.197 | 1.00 15.00 |
| ATOM | 771 | CA | LYS | 196 | -20.577 | 5.972 | 7.405 | 1.00 21.01 |
| ATOM | 772 | | LYS | 196 | -21.475 | 4.726 | 7.146 | 1.00 22.66 |
| ATOM | | CB | 113 175 | 196 | - 22 . 953 | 4 839 | 7.590 | 1.00 31.25 |
| ATOM | 773 | | 7.72 | 196 | -23.364 | 4.915 | 9.104 | 1.00 40.25 |
| ATOM | 774 | 35 | _ Y S _ Y S | 195 | -23.189 | 3.694 | 10.060 | 1.00 43.56 |
| ATOM | 775 | CE | LYS | 196 | -23.004 | 4.158 | 11.453 | 1.00 44.46 |
| ATOM | 776 | NZ | | | -22.182 | 4.799 | 11.467 | 1.00 15.00 |
| MCTA | 7 | HZI | | 196 | -23.847 | 4.665 | 11.778 | 1.00 15.00 |
| ATOM | 778 | HT2 | | 196 | -23.847 | 3.334 | 12.066 | 1.00 15.00 |
| ATOM | وحت | HZ3 | 7.32 | 196 | -22.50) | J. J.J. | 22.000 | |

FIGURE 17N

| ATOM | 780 | · c | LYS | 196 | -20.478 | 6.290 | 2 200 | | _ |
|------|-----|------|-----|-----|--------------------|--------|--------|------------|----|
| ATOM | 781 | | LYS | 196 | -20.194 | 5.434 | 8.899 | 1.00 19.25 | À |
| ATOM | 782 | | SER | 197 | -20.564 | 7.534 | 9.714 | 1.00 18.35 | À |
| ATOM | 753 | | SER | 197 | | | 9.272 | 1.00 20.63 | A |
| ATOM | | | | | -20.891 -20.752 | 8.247 | 8.615 | 1.00 15.00 | A |
| | 784 | | SER | 197 | | 7.701 | 10.729 | 1.00 24.87 | A |
| ATOM | 785 | | SER | 197 | -19.898 | 8.878 | 11.207 | 1.00 25.62 | A, |
| ATOM | 786 | | SER | 197 | -19.563 | 8.687 | 12.588 | 1.00 32.22 | A |
| ATOM | 787 | | SER | 197 | -18.795 | 8.110 | 12.611 | 1.00 15.00 | A |
| ATOM | 788 | C | SER | 197 | -22.216 | 7.810 | 11.218 | 1.00 26.33 | A |
| ATOM | 789 | 0 | SER | 197 | -23.078 | 8.303 | 10.497 | 1.00 26.57 | A |
| MOTA | 790 | N | PRO | 198 | -22.534 | 7.274 | 12.407 | 1.00 26.77 | A |
| ATOM | 791 | CD | PRO | 198 | -21.649 | 6.526 | 13.301 | 1.00 32.92 | A |
| ATOM | 792 | CA | PRO | 198 | -23.919 | 7.381 | 12.913 | 1.00 28.73 | A |
| ATOM | 793 | CB | PRO | 198 | -23.784 | 6.789 | 14.318 | 1.00 32.89 | A |
| ATOM | 794 | CG | PRO | 198 | -22.289 | 6.726 | 14.659 | 1.00 33.55 | A |
| ATOM | 795 | C | PRO | 198 | -24.591 | 8.789 | 12.847 | 1.00 26.60 | A |
| ATOM | 796 | 0 | PRO | 198 | -24.035 | 9.817 | 13.242 | 1.00 20.20 | A |
| ATOM | 797 | N | GLY | 199 | -25.729 | 8.773 | 12.119 | 1.00 25.75 | Ä |
| ATOM | 798 | Н | GLY | 199 | -26.170 | 7.857 | 12.057 | 1.00 15.00 | Ä |
| MOTA | 799 | CA | GLY | 199 | -26.486 | 10.003 | 11.790 | 1.00 26.91 | Â |
| ATOM | 800 | C | GLY | 199 | -25.821 | 10.971 | 10.816 | 1.00 28.98 | Ä |
| ATOM | 801 | ō | GLY | 199 | -26.084 | 12.151 | 10.797 | 1.00 31.05 | Ä |
| ATOM | 802 | N | ARG | 200 | -24.898 | 10.464 | 10.001 | 1.00 30.15 | |
| ATOM | 803 | Н | ARG | 200 | -24.629 | 9.519 | 10.165 | 1.00 15.00 | A |
| ATOM | 804 | CA | ARG | 200 | -24.140 | 11.384 | 9.166 | 1.00 28.98 | A |
| ATOM | 805 | CB | ARG | 200 | -22.749 | 11.590 | 9.783 | | A |
| ATOM | 806 | CS | ARG | 200 | -22.739 | 12.290 | 11.162 | 1.00 33.16 | A |
| ATOM | 807 | CD | ARG | 200 | -21.327 | 12.530 | | 1.00 38.34 | A |
| ATOM | 808 | NE | ARG | 200 | -21.292 | | 11.705 | 1.00 42.14 | A |
| ATOM | 809 | HE | ARG | 200 | -21.292 | 12.875 | 13.131 | 1.00 43.64 | A |
| ATOM | | CZ | | | | 13.831 | 13.424 | 1.00 15.00 | A |
| ATOM | 810 | | ARG | 200 | -21.138 | 11.896 | 14.051 | 1.00 46.40 | A |
| | 811 | | ARG | 200 | -21.219 | 10.603 | 13.733 | 1.00 46.31 | A |
| ATOM | 812 | HH11 | | 200 | -21.104 | 9.910 | 14.445 | 1.00 15.00 | A |
| ATOM | 813 | HH12 | | 200 | -21.394 | 10.320 | 12.789 | 1.00 15.00 | A |
| ATOM | 814 | | ARG | 200 | -20.901 | 12.226 | 15.311 | 1.00 46.65 | A |
| ATOM | | HH21 | | 200 | -20.847 | 13.193 | 15.566 | 1.00 15.00 | A |
| MOTA | 816 | HH22 | | 200 | -20.785 | 11.510 | 16.002 | 1.00 15.00 | A |
| ATOM | 817 | C | ARG | 200 | -24.084 | 10.967 | 7.710 | 1.00 27.77 | A |
| MCTA | 818 | С | ARG | 200 | -24.264 | 9.791 | 7.449 | 1.00 28.21 | Α |
| ATOM | 819 | N | PHE | 201 | -23.853 | 11.926 | 6.792 | 1.00 30.83 | A |
| ATOM | 82C | H | PHE | 201 | -23.513 | 12.821 | 7.126 | 1.00 15.00 | Α |
| MCTA | 821 | CA | PHE | 201 | -24.016 | 11.708 | 5.339 | 1.00 34.17 | A |
| MCTA | 922 | CB | PHE | 201 | -23.851 | 12.996 | 4.572 | 1.00 31.58 | A |
| ATOM | 823 | CG | PHE | 201 | -25.154 | 13.730 | 4.614 | 1.00 34.85 | A |
| MCTA | 824 | | PHE | 201 | | 15.062 | 5.081 | 1.00 37.56 | A |
| ATOM | 825 | | PHE | 201 | -26.335 | 13.081 | 4.190 | 7.00 37.89 | Α |
| ATOM | 826 | | PHE | 201 | -26.397 | 15.749 | 5.182 | 1.00 36.91 | Α |
| ATOM | 827 | CE2 | PHE | 201 | -27.566 | 13.762 | 4.280 | 1.00 38.98 | A |
| MCTA | 828 | CZ | PHE | 201 | -27.572 | 15.065 | 4.815 | 1.00 37.61 | Α |
| ATOM | 529 | C | PHE | 201 | -23.277 | 10.605 | 4.545 | 1.00 39.40 | Α |
| ATOM | 330 | 0 | PHE | 201 | -23.853 | 10.034 | 3.604 | 1.00 45.71 | A |
| ATOM | 831 | N | GLU | 202 | -22.031 | 10.316 | 5.034 | 1.00 35.75 | A |
| MOTA | 632 | H | GLU | 232 | -21.878 | 10.753 | 5.925 | 1.00 15.00 | A |
| ATOM | 833 | CA | GLU | 202 | -20.964 | 9.564 | 4.318 | 1.00 34.52 | A |
| ATOM | 834 | CB | SLU | 202 | -21.295 | 8.540 | 3.234 | 1.00 33.66 | A |
| ATCM | 835 | 23 | SLU | 202 | -21.924 | 7.245 | 3.713 | 1.00 40.61 | A |
| ATOM | 836 | 25 | SEU | 202 | -22.647 | 6.505 | 2.561 | 1.00 46.12 | Ä |
| ATOM | 837 | OE1 | SLU | 252 | -23.461 | 5.613 | 2.886 | 1.00 46.89 | A |
| ATOM | 535 | | SLU | 202 | -22.417 | 6.814 | 1.370 | 1.00 45.63 | Ä |
| ATOM | 839 | 3 | SLU | 202 | -19.924 | 10.450 | 3.717 | 1.00 29.99 | Â |
| | | - | | | £3.323 | 20.430 | J | | ~ |

FIGURE 170

| | 840 0 | GLU | 202 | -20.137 | 11.567 | 3.300 | 1.00 30.76 | A |
|--------------|-------------------------|-------|-----|---------|--------|--------|------------|-----|
| ATOM | 840 O 841 N | ARG | 203 | -18.728 | 9.897 | 3.856 | 1.00 26.88 | A |
| ATOM ATOM | 842 H | ARG | 203 | -18.690 | 8.998 | 4.285 | 1.00 15.00 | À |
| | 843 CA | ARG | 203 | -17.539 | 10.603 | 3.358 | 1.00 21.88 | Ä |
| ATOM ATOM | 844 CB | ARG | 203 | -16.819 | 11.410 | 4.457 | 1.00 27.07 | A |
| | 845 CG | ARG | 203 | -17.681 | 12.187 | 5.467 | 1.00 37.32 | A |
| ATOM | | ARG | 203 | -16.894 | 13.213 | 6.339 | 1.00 48.09 | · A |
| ATOM | 846 CD 847 NE | ARG | 203 | -15.911 | 12.667 | 7.308 | 1.00 56.90 | A |
| MOTA | | ARG | 203 | -16.240 | 12.433 | 8.223 | 1.00 15.00 | A |
| MOTA | | ARG | 203 | -14.572 | 12.475 | 7.001 | 1.00 66.77 | A |
| ATOM | | ARG | 203 | -13.702 | 12.002 | 7.911 | 1.00 68.44 | A |
| ATOM | 850 NH1 851 HH11 | | 203 | -12.745 | 11.829 | 7.666 | 1.00 15.00 | A |
| ATOM | | ARG | 203 | -14.016 | 11.822 | 8.845 | 1.00 15.00 | A |
| ATOM | | ARG | 203 | -14.084 | 12.716 | 5.766 | 1.00 67.68 | A |
| ATOM | | | 203 | -14.670 | 13.108 | 5.060 | 1.00 15.00 | A |
| ATOM | | ARG | 203 | -13.143 | 12.499 | 5.544 | 1.00 15.00 | Α |
| ATOM | | ARG | 203 | -16.517 | 9.633 | 2.678 | 1.00 17.71 | A |
| MOTA | 856 C | ARG | 203 | -16.375 | 8.418 | 2.931 | 1.00 7.69 | A |
| ATOM | 857 O 858 N | ILE | 204 | -15.789 | 10.253 | 1.791 | 1.00 14.42 | A |
| ATOM | | ILE | 204 | -15.915 | 11.228 | 1.561 | 1.00 15.00 | A |
| ATOM | | ILE | 204 | -14.662 | 9.482 | 1.353 | 1.00 18.32 | Α |
| ATOM | | ILE | 204 | -14.520 | 9.392 | -0.231 | 1.00 24.52 | Α |
| ATOM | | ILE | 204 | -15.820 | 9.529 | -1.069 | 1.00 21.85 | . A |
| MOTA | | ILE | 204 | -13.439 | 10.195 | -0.949 | 1.00 26.35 | A |
| ATOM | | | 204 | -13.992 | 11.231 | -1.961 | 1.00 36.33 | A |
| ATOM | | ILE | 204 | -13.387 | 9.819 | 2.153 | 1.00 16.58 | A |
| ATOM | 865 C | ILE | 204 | -13.070 | 10.956 | 2.457 | 1.00 18.63 | A |
| ATOM | 866 0 | LEU | 205 | -12.718 | 8.725 | 2.571 | 1.00 13.32 | A |
| ATOM | 867 N | LEU | 205 | -13.142 | 7.853 | 2.321 | 1.00 15.00 | A |
| ATOM | 868 H | LEU | 205 | -11.467 | 8.829 | 3.322 | 1.00 10.01 | Α |
| ATOM | 869 CA 870 CB | LEU | 205 | -11.440 | 7.688 | 4.382 | 1.00 6.66 | Α |
| MOTA | | LEU | 205 | -12.571 | 7.727 | 5.441 | 1.00 7.99 | Α |
| ATOM | | LEU | 205 | -12.722 | 9.088 | 6.089 | 1.00 8.78 | Α |
| ATOM | | LEU | 205 | -12.419 | 6.720 | 6.582 | 1.00 8.08 | A |
| ATOM | | LEU | 205 | -10.268 | 8.811 | 2.377 | 1.00 9.75 | Α |
| ATOM | 874 C | LEU | 205 | -9.416 | 9.655 | 2.320 | 1.00 10.25 | Α |
| ATOM | 875 O 876 N | LEU | 206 | -10.252 | 7.769 | 1.562 | 1.00 10.28 | A |
| ATOM | 876 N 877 H | LEU | 206 | -10.991 | 7.119 | 1.684 | 1.00 15.00 | Α |
| ATOM | 878 CA | LEU | 206 | -9.166 | 7.555 | 0.610 | 1.00 10.02 | A |
| ATOM | 879 CB | LEU | 206 | -8.249 | 6.384 | 0.990 | 1.00 11.94 | Α |
| ATOM | 880 CG | LEU | 206 | -7.001 | 6.527 | 1.859 | 1.00 14.40 | Α |
| ATOM | | LEU | 206 | -7.094 | 5.595 | 3.074 | 1.00 14.49 | Α |
| MOTA | | LEU | 206 | -6.531 | 7.958 | 2.151 | 1.00 8.78 | Α |
| ATOM ATOM | 883 C | LEU | 20€ | 9.756 | 7.071 | -0.697 | 1.00 11.91 | A |
| ATOM | 884 0 | LEU | 206 | -10.792 | 6.406 | -0.778 | 1.00 10.67 | Α |
| ATOM | 885 N | ARG | 207 | -9.005 | 7.428 | -1.720 | 1.00 8.06 | Α |
| ATOM | 886 H | ARG | 257 | -8.196 | 7.992 | -1.553 | 1.00 15.00 | A |
| ATOM | 88 CA | ARG | 207 | -9.309 | 6.823 | -2.992 | 1.00 10.45 | A |
| MOTA | 888 CB | ARG | 207 | -9.974 | 7.790 | -3.904 | 1.00 8.71 | A |
| ATOM | 889 CG | ARG | 207 | -11.258 | 8.270 | -3.357 | 1.00 15.68 | A |
| MOTA | 890 CD | ARG | 207 | -11.652 | 9.459 | -4.163 | 1.00 22.25 | A |
| ATOM | 891 NE | ARG | 207 | -12.670 | 9.192 | -5.171 | 1.00 29.59 | А |
| ATOM . | 892 HE | ARG | 207 | -13.115 | 8.300 | -5.249 | 1.00 15.00 | A |
| ATOM: | 893 CZ | ARG | 207 | -13.063 | 10.272 | -5.919 | 1.00 40.09 | A |
| ATOM | | ARG | 207 | -12.482 | 11.498 | -5.813 | 1.00 36.32 | A |
| ATOM | 895 HH1 | | 257 | -12.813 | 12.246 | -6.391 | 1.00 15.00 | A |
| ATOM | | ARS | 207 | -11.737 | 11.651 | -5.165 | 1.00 15.00 | A |
| ATOM | | 2 ARG | 207 | -14.067 | 10.111 | -6.773 | 1.00 40.86 | A |
| ATOM | | ARG | 207 | 14.392 | 10.877 | -7.329 | 1.00 15.00 | A |
| ATOM | 899 HH2 | | 207 | -14.498 | 9.207 | -6.853 | 1.00 15.00 | A |
| A.C | . | | - | | | | | |

FIGURE 17P

| | | | | | | | · |
|---|--|---|--|--|--|--|---|
| M ATTOM M M ATTOM M ATTOM M ATTOM M M M ATTOM M M M ATTOM M M M M ATTOM M M M M M ATTOM M M M M M M M M M M M M M M M M M M | 99999999999999999999999999999999999999 | ONHOCONHOCONHOCONHOCONHOCONHOCONHOCONHO | ASN ASN THR THR THR THR THR HIS HIS HIS HIS HIS SER R | 7775888899999900000000000000000000000000 | -2.043 -3.097 -3.097 -3.097 -3.097 -6.097 -6.298 -6.298 -6.298 -6.298 -6.298 -6.298 -6.298 -6.298 -6.298 -6.368 -7.468 -5.368 -6.37 | 6.456 -3.741 7.150 -3.787 5.358 -4.465 4.758 -4.355 5.128 -5.465 4.020 -5.072 4.830 -6.854 4.020 -7.057 5.586 -7.808 6.235 -7.533 5.208 -9.196 6.380 -10.069 4.461 -9.832 4.726 -9.593 3.491 -10.634 3.249 -10.531 2.893 -11.662 1.446 -11.355 1.366 -10.154 2.273 -9.342 0.165 -10.055 -0.479 -10.817 -0.081 -9.279 2.931 -13.043 2.752 -13.259 3.168 -14.013 3.377 -13.821 3.224 -15.314 4.158 -16.268 4.506 -17.438 5.493 -17.508 3.604 -16.581 1.833 -15.878 0.863 -15.475 1.718 -16.789 2.438 -16.878 0.863 -15.475 1.718 -16.789 2.438 -16.878 0.863 -15.475 1.718 -16.789 2.438 -16.878 0.454 -17.529 -0.012 -18.082 0.060 -17.111 0.967 -17.161 1.702 -17.794 -0.723 -15.985 -0.265 -15.383 0.780 -16.092 0.633 -18.683 -7.132 -19.443 2.323 -19.055 2.177 -20.675 2.704 -20.407 | 1.00 15.58 1.00 17.00 1.00 14.69 1.00 20.46 1.00 21.89 1.00 26.22 1.00 15.00 1.00 28.06 1.00 27.10 1.00 32.54 1.00 32.54 1.00 39.53 1.00 42.59 1.00 36.00 1.00 36.95 1.00 36.95 1.00 36.95 1.00 37.83 1.00 41.77 1.00 15.00 1.00 36.95 1.00 37.83 1.00 49.34 1.00 15.00 1.00 36.95 1.00 37.83 1.00 15.00 1.00 36.95 1.00 37.83 1.00 15.00 1.00 36.95 1.00 37.83 1.00 15.00 1.00 36.95 1.00 37.83 1.00 15.00 1.00 36.95 1.00 37.83 1.00 15.00 1.00 36.95 1.00 37.83 1.00 15.00 1.00 36.95 1.00 37.83 1.00 15.00 1.00 36.95 1.00 37.83 1.00 15.00 1.00 36.95 1.00 36.95 1.00 36.95 1.00 36.95 |
| | | | | | | | |
| | | | | 212 | | | |
| | | | | | | | |
| | | | | | | | |
| | | | | | | | |
| | 947 | н | SER | 213 | -7.156 | 2.323 -19.055 | |
| | | CA | | | | | |
| | | | | | | | - |
| ATOM | 950 | og | SER | 213 | -3.266 | 1.697 -20.547 | 1.00 53.97 |
| ATOM | 951 | HG | SER | 213 | -3.363 | 1.064 -19.823 | 1.00 15.00 |
| ATOM | 952 | C | SER | 213 | -5.844 | 1.508 -22.097 | |
| A.OM ATOM | 952 | | | | | | 1.00 60.03 |
| | | 0 | SER | 213 | -5.005 | 0.811 -22.682 | 1.00 61.19 |
| ATOM | 954 | N | SER | 214 | -7.043 | 1.803 -22.686 | 1.00 64.96 |
| ATOM | 955 | H. | SER | 214 | -7.705 | 2.322 -22.146 | 1.00 15.00 |
| ATOM | 956 | CA | SER | 214 | -7.463 | 1.456 -24.094 | 1.00 69.62 |
| ATOM | 957 | CB | SER | 214 | 8.727 | 2.218 -24.495 | 1.00 67.82 |
| ATOM | 958 | OG ::G | SER | 214 | -9.563 | 2.257 -23.336 | 1.00 67.64 |
| ATOM | 959 | нС | SER | 214 | -10.468 | 2.398 -23.623 | 1.00 15.00 |
| | | | | | | | |

FIGURE 17Q

| ATOM | 960 | C | SER | 214 | -6.518 | 1.587 | -25.300 | 1.00 | 72.08 | |
|--------|-------|------------------------|-----|-------|--------------------|---------|---------|--------|-------|--|
| ATOM | 961 | Š | SER | 214 | -6.102 | 2.683 | -25.686 | | 73.45 | |
| | 962 | N | ALA | . 215 | -6.175 | | -25.899 | | 73.3e | |
| ATOM | | | | 215 | -5.456 | | -26.565 | | 15.00 | |
| ATOM | 963 | H | ALA | | | | -25.753 | | 72.62 | |
| ATOM | 964 | CA | ALA | 215 | -6.858 | | | | | |
| ATOM | 965 | CB | ALA | 215 | -7.199 | | -27.138 | | 73.08 | |
| MOTA | 966 | C | ALA | 215 | -6.331 | -2.148 | -24.983 | | 72.11 | |
| MOTA | 967 | 0 | ALA | 215 | -7.020 | | -25.069 | | 72.74 | |
| MOTA | 968 | N | LYS | 216 | -5.153 | -2.076 | -24.282 | 1.00 | 70.17 | |
| ATOM | 969 | H | LYS | 216 | -4.747 | -1.165 | -24.199 | 1.00 | 15.00 | |
| ATOM | 970 | CA | LYS | 216 | -4.482 | -3.256 | -23.626 | 1.00 6 | 57.38 | |
| ATOM | 971 | CB | LYS | 216 | -3.458 | | -22.648 | | 55.30 | |
| ATOM | 972 | CG | LYS | 216 | -2.217 | | -23.321 | | 6.86 | |
| | 973 | CD | LYS | 216 | -1.419 | | -24.134 | 1.00 6 | | |
| ATOM | | | | | -0.082 | | -24.740 | | 7.51 | |
| ATOM | 974 | CE | LYS | 216 | | | | | | |
| ATOM | 975 | NZ | LYS | 216 | 0.483 | | -25.598 | | 7.80 | |
| ATOM | 976 | HZ1 | LYS | 216 | 0.620 | | -25.041 | | 15.00 | |
| ATOM | 977 | HZ2 | LYS | 216 | -0.168 | | -26.385 | | 15.00 | |
| ATOM | 978 | HZ3 | LYS | 216 | 1.401 | -3.406 | -25.973 | 1.00 | .5.00 | |
| ATOM | 979 | C | LYS | 216 | -5.321 | -4.441 | -22.993 | 1.00 € | 66.99 | |
| ATOM | 980 | 0 | LYS | 216 | -6.462 | -4.266 | -22.575 | 1.00 € | 9.90 | |
| ATOM | 981 | N | PRO | 217 | -4.835 | -5.724 | -22.952 | 1.00 6 | 5.06 | |
| ATOM | 982 | CD | PRO | 217 | -3.525 | -6.262 | -23.308 | 1.00 € | 7.91 | |
| ATOM | 983 | CA | PRO | 217 | -5.792 | | -22.626 | | 2.80 | |
| | | CB | PRO | 217 | -5.285 | | -23.464 | 1.00 6 | | |
| ATOM | 984 | | | | -3.755 | -7.799 | -23.338 | | 9.63 | |
| ATOM | 985 | CG | PRO | 217 | | | | 1.00 5 | | |
| MOTA | 986 | C | PRO | 217 | -5.837 | | -21.150 | | | |
| ATOM | 987 | 0 | PRO | 217 | -4.747 | | -20.589 | | 8.81 | |
| ATOM | 988 | N | CYS | 218 | -7.115 | | -20.627 | | 55.45 | |
| MOTA | 989 | H | CYS | 218 | -7.874 | | -21.233 | | 5.00 | |
| ATOM | 990 | CA | CYS | 218 | -7.433 | -7.929 | -19.210 | 1.00 4 | | |
| MCTA | 991 | CB | CYS | 218 | -8.105 | -9.289 | -19.079 | 1.00 4 | | |
| ATOM | 992 | SG | CYS | 218 | -8.855 | -9.822 | -17.460 | 1.00 4 | 3.11 | |
| ATOM | 993 | С | CYS | 218 | -6.265 | -7.994 | -18.263 | 1.00 4 | 3.24 | |
| ATOM | 994 | ō | CYS | 218 | -5.720 | -9.026 | -17.959 | 1.00 4 | 4.68 | |
| ATOM | 995 | N | GLY | 219 | -5.853 | -6.820 | -17.876 | | 0.28 | |
| | 996 | Н | GLY | 219 | -6.328 | -5.961 | -18.059 | | 5.00 | |
| ATOM | | | GLY | 219 | -4.659 | -6.828 | -17.070 | | 6.27 | |
| ATOM | 997 | CA | | | -5.017 | | -15.643 | | 3.86 | |
| ATOM | 998 | C | GLY | 219 | | | | | | |
| ATOM | 999 | 0 | GLY | 219 | -5.906 | -6.452 | -15.097 | | 34.90 | |
| MCTA | 1000 | N | GLN | 220 | -4.313 | -7.996 | -15.023 | | 3.15 | |
| ATOM | 1001 | Н | GLN | 220 | -3.835 | -8.684 | -15.580 | | 5.00 | |
| ATOM | 1002 | CA | GLN | 220 | -4.448 | | -13.578 | | 9.92 | |
| ATOM | 1003 | CB | GLN | 220 | -4.298 | | -12.936 | 1.00 2 | 7.81 | |
| ATOM | 1004 | CG | GLN | 220 | -5.380 | -9.340 | -11.883 | | 10.94 | |
| ATOM | 1005 | CD | GLN | 220 | -5.285 | -10.631 | -11.132 | 1.00 3 | 36.37 | |
| ATOM | 1006 | | GLN | 220 | | -10.969 | | 1.00 3 | 88.47 | |
| MOTA | 1007 | | GLN | 220 | | -11.296 | | 1.00 | 37.61 | |
| ATOM | 1008 | HE21 | | 220 | | -12.235 | | 1.00 | | |
| | | | | | -7.373 | -11.036 | | 1.00 | | |
| ATOM | 1009 | HE22 | | 220 | | | -12.859 | 1.00 | | |
| ATOM | 1010 | C | GLN | 220 | -3.666 | | -12.999 | 1.00 | | |
| MOTA | 1011 | 0 | GLN | 223 | -2.461 | | | | | |
| MOTA | 1012 | N | GLN | 221 | -4.438 | | -12.110 | 1.00 | | |
| ATOM : | .1013 | H | GLN | 221 | -5.433 | | -12.143 | 1.00 | | |
| ATOM | 1014 | CA | GLN | 221 | -3.803 | | -11.387 | 1.00 | | |
| MCTA | 1015 | CB | GLN | 221 | -4.077 | | -11.949 | 1.00 | | |
| MOTA | 1016 | CG | GLN | 221 | -3.284 | | -13.163 | 1.00 | | |
| MCTA | 1017 | $\mathbb{C}\mathbb{D}$ | GLN | 221 | -3.795 | | -13.405 | 1.00 | | |
| ATOM | 1018 | OE: | GLN | 221 | -3.746 | | -12.558 | 1:00 4 | 12.12 | |
| MCTA | 1019 | NE2 | GLN | 221 | -4.648 | -1.507 | -14.398 | 1.00 | 34.93 | |
| | | | | | · · · · | | | | | |

FIGURE 17R

| | 1020 | 11501 | GLN | 221 | -4.9 | 81 . | -2.187 | -15.042 | 1.00 | 15.00 |
|--------|------|-------|-------|-----|---------|------|--------|---------|------|---------------|
| MOTA | | | | | - 4 . 8 | | -0.551 | -14.575 | 1.00 | 15.00 |
| ATOM | 1021 | HE22 | GLN | 221 | | - | | -9.948 | 1.00 | 19.54 |
| MCTA | 1022 | C | GLN . | 221 | -4.2 | | -4.913 | | | |
| MOTA | 1023 | 0 | GLN | 221 | -5.3 | | -5.381 | -9.611 | 1.00 | 19.46 |
| ATOM | 1024 | N | SER | 222 | -3.3 | | -4.330 | -9.123 | 1.00 | 15.12 |
| MOTA | 1025 | Н | SER | 222 | -2.4 | 42 - | -4.098 | -9.441 | 1.00 | 15.00 |
| | | CA | SER | 222 | -3.8 | | -4.120 | -7.752 | 1.00 | 19.45 |
| MOTA | 1026 | | | | -3.1 | | -4.947 | -6.691 | 1.00 | 19.99 |
| ATOM | 1027 | CB | SER | 222 | | | -6.339 | -7.053 | | 24.64 |
| ATOM | 1028 | OG | SER | 222 | -3.0 | | | | | 15.00 |
| ATOM | 1029 | HG | SER | 222 | -2.6 | | -6.336 | -7.904 | _ | |
| ATOM | 1030 | C | SER | 222 | -3.7 | | -2.688 | -7.330 | | 24.09 |
| ATOM | 1031 | 0 | SER | 222 | -2.9 | | -1.929 | -7.944 | | 29.41 |
| ATOM | 1032 | N | ILE | 223 | -4.5 | 34 . | -2.386 | -6.283 | 1.00 | 22.81 |
| | 1033 | н | ILE | 223 | -5.1 | 72 - | -3.127 | -6.074 | 1.00 | 15.00 |
| ATOM | | | ILE | 223 | -4.5 | | -1.122 | -5.530 | 1.00 | 21.06 |
| ATOM | 1034 | CA | | | -5.9 | | -0.490 | -5.852 | | 19.87 |
| ATOM | 1035 | CB | ILE | 223 | | | | | | 16.59 |
| ATOM | 1036 | CG2 | ILE | 223 | -6.5 | | 0.315 | -4.673 | | |
| ATOM | 1037 | CG1 | ILE | 223 | -5.9 | | 0.278 | -7.188 | | 15.22 |
| ATOM | 1038 | CD1 | ILE | 223 | -7.2 | 29 | 0.868 | -7.709 | | 20.54 |
| ATOM | 1039 | Č | ILE | 223 | -4.3 | 67 | -1.446 | -4.007 | 1.00 | 21.62 |
| | | ŏ | ILE | 223 | -5.0 | 98 | -2.269 | -3.444 | 1.00 | 19.58 |
| MOTA | 1040 | | | | -3.4 | | -0.767 | -3.340 | | 19.73 |
| MOTA | 1041 | N | HIS | 224 | | | -0.230 | -3.899 | | 15.00 |
| ATOM | 1042 | H | HIS | 224 | -2.7 | | | | | |
| ATOM | 1043 | CA | HIS | 224 | -3.4 | | -0.671 | -1.858 | | 16.45 |
| ATOM | 1044 | CB | HIS | 224 | -2.1 | | -1.183 | -1.227 | 1.00 | |
| ATOM | 1045 | CG | HIS | 224 | -2.1 | 82 - | -1.442 | 0.296 | | 14.92 |
| MOTA | 1046 | ND1 | | 224 | -2.4 | 79 - | -2.628 | 0.582 | 1.00 | 15.33 |
| | | | HIS | 224 | -2.6 | | -3.515 | 0.505 | 1.00 | 15.00 |
| ATOM | 1047 | HD1 | | | -1.9 | | -0.524 | 1.310 | | 13.79 |
| MOTA | 1048 | _ | HIS | 224 | | | | 2.517 | | 10.52 |
| MOTA | 1049 | NE2 | HIS | 224 | -2.1 | | -1.127 | | | |
| MOTA | 1050 | CE1 | HIS | 224 | -2.4 | | -2.411 | 2.232 | | 11.70 |
| MOTA | 1051 | С | HIS | 224 | -3.9 | 14 | 0.699 | -1.284 | 1.00 | |
| ATOM | 1052 | Õ | HIS | 224 | -3.3 | 38 | 1.732 | -1.520 | 1.00 | 14.36 |
| ATOM | 1053 | N | LEU | 225 | -4.9 | 70 | 0.673 | -0.468 | 1.00 | 16.85 |
| | | | LEU | 225 | -5.3 | | -0.238 | -0.252 | 1.00 | 15.00 |
| MOTA | 1054 | H | | 225 | -5.3 | | 1.885 | 0.256 | 1.00 | 15.55 |
| MOTA | 1055 | CA | LEU | | | | 2.082 | 0.208 | | 17.15 |
| ATOM | 1056 | CB | LEU | 225 | -6.9 | | | -1.154 | | 18.03 |
| ATOM | 1057 | CG | LEU | 225 | -7.4 | | 2.456 | | | |
| MCTA | 1058 | CD1 | LEU | 225 | -6.7 | | 3.659 | -1.774 | | 19.34 |
| MOTA | 1059 | CD2 | LEU | 225 | -8.9 | 94 | 2.659 | -1.098 | | 13.66 |
| ATOM | 1060 | C | LEU | 225 | -5.0 | 74 | 1.758 | 1.739 | 1.00 | 14.77 |
| | 1061 | Ö | LEU | 225 | -5.3 | 47 | 0.726 | 2.345 | 1.00 | 12.20 |
| ATOM | | | GLY | 226 | -4.5 | | 2.829 | 2.344 | 1.00 | 18.04 |
| ATOM | 1062 | N | | | -4.2 | | 3.616 | 1.813 | 1.00 | 15.00 |
| ATOM | 1063 | H | GLY | 226 | | | 2.833 | 3.841 | | 18.37 |
| MOTA | 1064 | CA | GLY | 226 | -4.5 | | | | | |
| ATOM | 1065 | C | GLY | 226 | -4.1 | | 4.171 | 4.544 | | 17.08 |
| ATOM | 1066 | 0 | GLY | 226 | - 3 . 3 | 89 | 4.906 | 4.055 | | 13.75 |
| ATOM | 1067 | N | GLY | 227 | -4.7 | 781 | 4.457 | 5.725 | | 16.30 |
| ATOM | 1068 | Н | GLY | 227 | -5.4 | 34 | 3.771 | 6.036 | 1.00 | 15.00 |
| | | CA | GLY | 227 | -4.3 | | 5.649 | 6.490 | 1.00 | 8.52 |
| ATOM | 1069 | | | 227 | -4.9 | | 5.631 | 7.959 | 1.00 | 12.75 |
| ATOM | 1070 | C | GLY | | | | 4.748 | 8.466 | 1.00 | 10.57 |
| ATOM | 1071 | 0 | GLY - | 227 | -5.6 | | 6.698 | 8.675 | 1.00 | 9.23 |
| ATOM . | 1072 | N | VAL | 228 | -4.5 | | | | 1.00 | 15.00 |
| MOTA | 1073 | H | VAL | 228 | -4.0 | | 7.398 | 8.222 | | |
| MOTA | 1074 | CA | VAL | 228 | - 5 . 1 | | 6.818 | 10.067 | | 11.74 |
| ATOM | 1075 | CB | VAL | 228 | -4.0 | 285 | 7.320 | 11.144 | 1.00 | 14.30 |
| ATOM | 1076 | | | 228 | -2.8 | 330 | 6.445 | 11.333 | | 10.73 |
| | 1377 | | | 228 | -4.7 | | 7.565 | 12.479 | 1.00 | |
| ATOM | | | VAL | 228 | -6.2 | | 7.803 | 10.098 | 1.00 | 9.03 |
| MOTA | 1078 | | | | -6.0 | | 8.937 | _ | | 12.01 |
| ATOM | 1079 | 0 | VAL | 228 | - 0 . (| 009 | 0.931 | | 2.00 | · |

FIGURE 17S

| 2 7 2 14 | 1080 | N | PHE | . 229 | -7.347 | 7.299 | 10.640 | 1.00 9.88 |
|----------|--------------|----------|------|-------|------------|--------|--------|------------|
| ATOM | | H | PHE | 229 | -7.329 | 6.332 | 10.922 | 1.00 15.00 |
| MOTA | 1081 | | | | -8.566 | 8.106 | 10.772 | 1.00 11.18 |
| ATOM | 1082 | CA | PHE | 229 | | 7.687 | 9.686 | 1.00 8.01 |
| MCTA | 1083 | CB | PHE | 229 | -9.578 | | | 1.00 8.40 |
| ATOM | 1084 | CG | PHE | 229 | -9.063 | 7.912 | 8.233 | |
| MCTA | 1085 | CD1 | PHE | 229 | -9.140 | 9.196 | 7.649 | 1.00 10.03 |
| MOTA | 1086 | CD2 | PHE | 229 | -8.433 | 6.883 | 7.517 | 1.00 6.57 |
| ATOM | 1087 | CEl | PHE | 229 | -8.512 | 9.443 | 6.395 | 1.00 5.18 |
| | | CE2 | PHE | 229 | -7.771 | 7.128 | 6.282 | 1.00 4.26 |
| ATOM | 1088 | | PHE | 229 | -7.813 | 8.424 | 5.731 | 1.00 5.71 |
| ATOM | 1089 | CZ | | | -9.202 | 8.014 | 12.197 | 1.00 14.39 |
| ATOM | 1090 | Ç | PHE | 229 | | | 12.870 | 1.00 13.92 |
| MOTA | 1091 | 0 | PHE | 229 | -9.116 | 7.000 | | 1.00 17.93 |
| ATOM | 1092 | N | GLU | 230 | -9.863 | 9.064 | 12.672 | |
| ATOM | 1093 | Н | GLU | 230 | -9.912 | 9.892 | 12.113 | 1.00 15.00 |
| ATOM | 1094 | CA | GLU | 230 | -10.856 | 8.944 | 13.770 | 1.00 18.08 |
| ATOM | 1095 | CB | GLU | 230 | -11.218 | 10.303 | 14.393 | 1.00 16.17 |
| ATOM | 1096 | ĊĠ | GLU | 230 | -11.068 | 10.090 | 15.889 | 1.00 27.69 |
| | 1097 | CD | GLU | 230 | -12.314 | 10.091 | 16.805 | 1.00 33.06 |
| MOTA | | OE1 | | 230 | -13.355 | 10.707 | 16.552 | 1.00 38.26 |
| ATOM | 1098 | | | | -12.218 | 9.477 | 17.863 | 1.00 38.14 |
| ATOM | 1099 | | GLU | 230 | | | 13.453 | 1.00 18.70 |
| MOTA | 1100 | С | GLU | 230 | -12.225 | 8.268 | | 1.00 21.58 |
| MOTA | 1101 | 0 | GLU | 230 | -12.967 | ε.519 | 12.492 | |
| MOTA | 1102 | N | LEU | 231 | -12.542 | 7.334 | 14.361 | 1.00 13.79 |
| MOTA | 1103 | Н | LEU | 231 | -11.840 | 7.125 | 15.015 | 1.00 15.00 |
| ATOM | 1104 | CA | LEU | 231 | -13.885 | 6.836 | 14.330 | 1.00 13.52 |
| ATOM | 1105 | CB | LEU | 231 | -13.954 | 5.378 | 14.002 | 1.00 13.90 |
| ATOM | 1103 | CG | LEU | 231 | -13.199 | 5.064 | 12.725 | 1.00 15.44 |
| ATOM | 1107 | | LEU | 231 | -13.781 | 5.712 | 11.436 | 1.00 10.24 |
| MCTA | 1108 | | LEU | 231 | -12.970 | 3.569 | 12.769 | 1.00 11.74 |
| | 1109 | c | LEU | 231 | -14.638 | 7.074 | 15.591 | 1.00 14.88 |
| ATOM | | | LEU | 231 | -14.145 | 6.912 | 16.692 | 1.00 12.46 |
| ATOM | 1110 | 0 | | | -15.891 | 7.411 | 15.350 | 1.00 19.40 |
| ATOM | 1111 | N | GLN | 232 | -16.107 | 7.560 | 14.394 | 1.00 15.00 |
| ATOM | 1112 | H | GLN | 232 | | 7.509 | 16.389 | 1.00 21.07 |
| ATOM | 1113 | CA | GLN | 232 | -16.920 | | | 1.00 23.55 |
| ATOM | 1114 | CB | GLN | 232 | -18.132 | 8.234 | 15.804 | |
| ATOM | 1115 | CG | GLN | 232 | -17.792 | 9.709 | 15.687 | 1.00 28.60 |
| ATOM | 1116 | CD | GLN | 232 | -17.625 | 10.200 | 17.102 | 1.00 33.66 |
| ATOM | 1117 | OEl | GLN | 232 | -18.623 | 10.472 | 17.742 | 1.00 38.08 |
| ATOM | 1118 | NE2 | GLN | 232 | -16.380 | 10.254 | 17.596 | 1.00 33.41 |
| ATOM | | HE21 | GLN | 232 | -15.596 | 10.186 | 16.972 | 1.00 15.00 |
| ATOM | | HE22 | GLN | 232 | -16.387 | 10.470 | 18.576 | 1.00 15.00 |
| ATOM | 1121 | C | GLN | 232 | -17,402 | 6.148 | 16.851 | 1.00 21.86 |
| ATOM | 1122 | Ö | GLN | 232 | -17.368 | 5.218 | 16.052 | 1.00 21.58 |
| ATOM | 1123 | N | PRO | 233 | -17.906 | 6.013 | 18.115 | 1.00 22.31 |
| | 1123 | CD | PRO | 233 | -17,962 | 7.033 | 19.168 | 1.00 21.41 |
| ATOM | 1124 1125 | | PRC | 232 | -18.570 | 4.747 | 18.442 | 1.00 21.21 |
| ATOM | | CA | | | -19.013 | 4.987 | 19.866 | 1.00 23.88 |
| MCTA | 1126 | CB | 220 | 233 | -18.661 | 6.404 | 20.339 | 1.00 20.95 |
| ATOM | 1127 | CG | PRO | 233 | | 4.417 | 17.434 | 1.00 23.66 |
| ATOM | 1128 | Ę | PRO | 233 | -19.667 | | 16.875 | 1.00 26.89 |
| ATOM | 1129 | 0 | PRO | 233 | - 20 . 275 | 5.319 | | |
| ATCM | 1129 | N | SLY | 234 | -19.731 | 3.140 | 17.059 | 1.00 22.77 |
| ATOM | | Н | GLY | 234 | -19.082 | 2.466 | 17.417 | 1.00 15.00 |
| ATOM . | 1132 | CA | GLY | 234 | -20.766 | 2.767 | 16.072 | 1.00 19.45 |
| ATOM | 11133 | 2 | SLY | 234 | -20.545 | 3.241 | 14.625 | 1.00 19.67 |
| ATCM | 1.34 | : | 51.X | 234 | -21.299 | 2.980 | 13.715 | 1.00 23.81 |
| ATOM | 1 1 5 5 | : :: | ALA | 235 | -19.405 | 3.926 | 14.368 | 1.00 18.89 |
| ATOM | 1136 | : H | ALA | 235 | -19.096 | 4.485 | 15.135 | 1.00 15.00 |
| ATOM | 1137 | CA | ÄLÄ | 235 | -18.431 | 3.515 | 13.296 | 1.00 22.17 |
| ATOM | 1138 | CB | ALA | 235 | -18.193 | 2.042 | 13.039 | 1.00 6.68 |
| | 1139 | 3 | ٨٠٨ | 235 | -18.540 | 4.160 | 11.993 | 1.00 21.96 |
| ATOM | | - | ~~~ | | 20.2.0 | | | |

FIGURE 17T

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12.100 1.00 5.385 26.42 235 -18.486 متم 1140 ATOM 1.50 20.94 -18.699 3.498 ATOM 1141 N SER 236 15.00 17.60 10.254 4.326 236 -18.524 ATOM SER 1142 2.227 9.961 1.00 -18.630 236 1143 SER ATOM 1.00 14.96 СВ -19.905 1.876 9.160 SER 236 1144 ATOM 1.00 -20.662 0.908 9.833 1145 OG SER 236 ATOM 1.00 15.00 0.910 9.647 -21.599 SER 236 HG MCTA 1146 -17.794 1.00 13.65 2.538 8.714 SER 23€ 1147 ATOM -17.939 8.131 1.00 16.29 3.614 236 SER ATOM 1148 0 1.00 14.95 1.567 8.286 237 -16:986 N VAL 1149 ATOM 15.00 -16.764 1.00 0.823 8.949 237 1150 Η VAL MOTA 11.42 1.00 237 -16.201 1.802 7.077 VAL 1151 CA ATOM 7.284 1.00 12.49 2.004 -14.681 CB VAL 237 1152 ATOM 1.00 13.10 -14.113 0.726 7.939 VAL 237 1153 CG1 ATOM 1.00 10.27 237 3.396 7.846 VAL -14.254 ATOM 1154 CG2 1.00 6.035 8.76 0.746 -16.468 VAL 237 1155 C **ATOM** 1.00 12.84 -16.827 -0.363 6.341 1156 VAL 237 0 MOTA 1.00 12.45 4.773 1.158 -16.354 ATOM 1157 N PHE 238 1.00 15.00 -16.139 2.128 4.652 PHE 238 1158 Н ATOM 3.653 1.00 11.21 0.213 -16.521 PHE 238 1159 CA MOTA 1.00 13.00 -18.013 0.137 3.322 23B CB PHE ATOM 1160 2.899 1.00 12.17 1.468 CG PHE 238 -18.634 MOTA 1161 1.518 1.00 12.94 -18.763 1.812 CD1 1162 PHE 238 ATOM 1.00 10.55 3.887 CD2 PHE 238 -19.135 2.332 1163 ATOM 1.092 1.00 14.01 3.010 CEl -19.407 1164 PHE 238 MCTA -19.786 3.504 3.470 1.00 12.74 CE2 PHE 238 1165 MCTA 1.00 13.17 2.100 -19.917 3.836 238 1166 CZ PHE MCTA 0.582 2.379 1.00 11.20 -15.725 \subset PHE 238 MCTA 1167 1.00 8.73 -15.137 1.638 2.267 238 0 PHE ATOM 1168 1.00 14.34 -15.726 1.383 VAL 239 -0.300 ATOM 1169 N 1.00 15.00 -1.170 -16.187 1.523 VAL 239 1170 Н MCTA 1.00 14.65 0.027 0.154 -14.982 VAL 1171 CA 239 MCTA 1172 1173 1174 1.00 14.09 -13.900 -1.043 -0.162 239 VAL CB ATOM 1.00 14.55 -13.004 -1.318 1.038 CG1 VAL 239 MCTA -0.594 -1.361 1.00 14.74 -13.064 VAL 239 ATOM CGZ 1.00 18.32 -1.043 VAL 239 -15.930 0.081 1175 C ATCM -0.903 -1.369 1.00 18.99 1176 -16.558 VAL 239 0 MCTA 1.00 19.26 -16.000 1.207 -1.707 240 1177 N ASN ATOM -1.383 1.00 15.00 1.947 1178 -15.420 ASN 240 Н ATOM -3.031 1.00 21.66 -16.613 1.355 240 1179 CA ASN MCTA 1.00 24.58 -16.850 2.856 -3.095 240 CB ASN 1180 MCTA 3.077 -3.708 1.00 29.09 -18.167 ASN 240 ATOM 1181 CG -3.740 1.00 35.44 -18.948 2.123 1182 ODI ASN 240 ATOM 1.00 34.71 -4.166 -18.293 4.331 240 ATOM ND2 ASN 1193 4.489 -4.657 1.00 15.00 -19.149 1184 ASN 240 HD21 ATOM 0.950 -4.184 1.00 20.96 -15.669 1155 ASN 240 ATOM 1.00 20.99 -4.058 -14.473 1-128 240 ATOM 0 ASN 1186 -5.275 1.00 21.52 0.383 -16.189 VAL 241 1187 N ATOM 1.00 15.00 -5.295 -17.182 0.230 ATCM 241 1188 VAL H -6.516 1.00 20.56 0.439 1189 VAL 241 -15.387 CA ATOM -14.581 -0.850 -6.849 1.00 18.02 241 ATCM 1190 CB VAL 1.00 15.06 -7.063 -2.058 -15.501 VAL 241 1191 CG1 ATOM -5.764 1.00 20.05 -13.597 -1.259 VAL 1192 241 CG2 ATOM -7.741 1.00 18.88 -16.253 0.758 1193 VAL 241 ATOM -7.819 1.00 18.53 0.500 -17.441 24: ∵a_ ATCM -B.762 1.00 21.24 -15.541 1.162 1195 242 ATOM THR 1.00 15.00 -8.486 -14.704 1.653 1196 THR 242 ATOM 1.00 20.63 -10.031 THR 1197 242 -16.246 1.476 ATOM 1.00 15.80 2.269 -10.981 -15.342 ATCM 242 1198 CB THR 1.00 17.72 1.663 -10.953

-14.035

242

1199

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FIGURE 17U

| - | | | | 2.4.2 | | 1.969 - | 11.812 | 1.00 15.00 |
|------|--------------|-----------|-----|-------|---------|------------------|--------|------------|
| MCTA | 1200 | HG1 | THR | 242 | -13.721 | | 10.650 | 1.30 15.34 |
| ATOM | 1201 | CG2 | THR | 242 | -15.238 | | | |
| ATOM | 1202 | \subset | THR | 242 | -16.755 | | 10.783 | 1.00 15.92 |
| ATOM | 1203 | С | THR | 242 | -17.846 | | 11.297 | 1.00 21.26 |
| ATOM | 1204 | N | ASP | 243 | -15.923 | | 10.718 | 1.00 20.98 |
| ATOM | 1205 | H | ASP | 243 | -15.087 | | 10.221 | 1.00 15.00 |
| ATOM | 1206 | CA | ASP | 243 | -16.092 | -1.977 - | 11.628 | 1.00 21.28 |
| ATOM | 1207 | CB | ASP | 243 | -14.905 | -2.126 - | 12.594 | 1.00 22.05 |
| ATOM | 1208 | ĊĠ | ASP | 243 | -14.932 | -0.954 - | 13.492 | 1.00 28.23 |
| | 1200 | 001 | ASP | 243 | -14.314 | | 13.115 | 1.00 28.43 |
| MOTA | | | ASP | 243 | -15.588 | | 14.535 | 1.00 33.00 |
| ATOM | 1210 | | | | | | 10.923 | 1.00 20.38 |
| ATOM | 1211 | C | ASP | 243 | -16.123 | | | |
| ATOM | 1212 | 0 | ASP | 243 | -15.148 | | 10.967 | 1.00 20.43 |
| ATOM | 1213 | N | PRO | 244 | -17.204 | | 10.154 | 1.00 19.92 |
| MOTA | 1214 | CD | PRO | 244 | -18.481 | -2.871 - | | 1.00 16.83 |
| ATOM | 1215 | CA | PRO | 244 | -17.120 | -4.706 | -9.269 | 1.00 19.13 |
| ATOM | 1216 | CB | PRO | 244 | -18.293 | -4.535 | -8.275 | 1.00 15.33 |
| ATOM | 1217 | CG | PRO | 244 | -18.890 | -3.174 | -8.634 | 1.00 15.21 |
| ATOM | 1218 | C | PRO | 244 | -16.975 | -6.034 | -9.974 | 1.00 19.29 |
| ATOM | 1219 | 0 | PRO | 244 | -16.194 | | -9.548 | 1.00 23.48 |
| | | | SER | 245 | -17.581 | -6.163 - | | 1.00 22.60 |
| ATOM | 1220 | N | | | -18.220 | | 11.473 | 1.00 15.00 |
| ATOM | 1221 | H | SER | 245 | | -7.429 - | | 1.00 25.50 |
| ATOM | 1222 | CA | SER | 245 | -17.414 | | _ | 1.00 23.36 |
| ATOM | 1223 | CB | SER | 245 | -18.256 | | 13.234 | |
| MOTA | 1224 | OG | SER | 245 | -19.667 | | 12.981 | 1.00 38.26 |
| ATOM | 1225 | HG | SER | 245 | -19.848 | -7.390 - | | 1.00 15.00 |
| ATOM | 1226 | С | SER | 245 | -15.955 | -7.7 76 - | 12.328 | 1.00 24.14 |
| ATOM | 1227 | 0 | SER | 245 | -15.477 | | 12.623 | 1.00 24.84 |
| ATOM | 1228 | N | GLN | 246 | -15.177 | -6.689 - | 12.385 | 1.00 28.52 |
| ATOM | 1229 | н | GLN | 246 | -15.638 | -5.804 - | 12.265 | 1.00 15.00 |
| ATOM | 1230 | CA | GLN | 246 | -13.743 | | 12.590 | 1.00 26.45 |
| | 1231 | CB | GLN | 246 | -13.144 | -5.645 - | | 1.00 29.90 |
| ATOM | | | GLN | 246 | -13.403 | | 14.758 | 1.00 26.84 |
| ATOM | 1232 | CG | | | -14.862 | -5.341 - | | 1.00 21.60 |
| MCTA | 1233 | CD | GLN | 246 | | | 14.616 | 1.00 24.20 |
| ATOM | 1234 | OEl | GLN | 246 | -15.538 | | | 1.00 24.20 |
| ATOM | 1235 | NE2 | GLN | 246 | -15.334 | | 15.975 | |
| ATOM | 1236 | HE21 | GLN | 246 | -14.763 | | 16.423 | 1.00 15.00 |
| MOTA | 1237 | HE22 | GLN | 246 | -16.320 | | 16.084 | 1.00 15.00 |
| ATOM | 1238 | C | GLN | 246 | -12.936 | | 11.363 | 1.00 27.14 |
| ATOM | 1239 | 0 | GLN | 246 | -11.721 | -7.570 - | 11.454 | 1.00 25.73 |
| MCTA | 1240 | N | VAL | 247 | -13.615 | -7.395 - | 10.196 | 1.00 23.70 |
| ATOM | 1241 | Н | VAL | 247 | -14.600 | -7.594 - | 10.146 | 1.00 15.00 |
| ATOM | 1242 | CA | VAL | 247 | -12.728 | -7.569 | -9.097 | 1.00 21.91 |
| ATOM | 1243 | CB | VAL | 247 | -13.156 | -6.814 | -7.859 | 1.00 21.59 |
| | | | | 247 | -14.027 | -7.616 | | 1.00 24.52 |
| ATOM | 1244 | CG1 | VAL | 247 | 13 690 | -5 409 | -8.167 | 1.00 21.61 |
| MOTA | 1245 | | VAL | | | | -8.910 | 1.00 21.55 |
| ATOM | 1246 | C | VAL | 247 | -12.258 | | 9.251 | 1.00 19.53 |
| MOTA | 1247 | 0 | VAL | 247 | -12.946 | | | |
| ATOM | 1248 | N | SER | 248 | -11.000 | -9.152 | -8.444 | 1.00 21.31 |
| ATOM | 1249 | Н | SER | 248 | -10.558 | -8.342 | -8.070 | 1.00 15.00 |
| ATOM | 1250 | CA | SER | 248 | -10.414 | -10.499 | -8.327 | 1.00 21.97 |
| ATOM | 1251 | CB | SER | 248 | -8.939 | -10.571 | -8.828 | 1.00 23.61 |
| MCTA | 1252 | 03 | SER | 248 | | -9.952 - | | 1.00 20.21 |
| ATOM | 1252 | HG | SER | 248 | -9.752 | -10.027 - | 10.496 | 1.00 15.00 |
| ATCM | 1254 | 2 | SER | 248 | -10.538 | | -6.946 | 1.00 19.28 |
| ATOM | | Š | SER | 248 | -10.048 | -10.409 | -6.052 | 1.00 20.64 |
| ATOM | 1255 1256 | Ň | HIS | 249 | -11.269 | | -6.814 | 1.00 18.72 |
| | | | | 249 | | -12.753 | -7.674 | 1.00 15.00 |
| ATOM | 1257 | H | #15 | | 540 | -12.673 | -5.478 | 1.00 17.22 |
| ATOM | 1258 | CA | HIS | 249 | | -13.152 | -5.484 | 1.00 17.22 |
| ATOM | 1259 | CB | HIS | 249 | 3.060 | -13.134 | J. 404 | 1.00 13.10 |
| | | | | | | | | |

FIGURE 17V

| | | | | idone | | • | |
|-------|------|---------|-----|----------------------------|--------|------------|-----|
| | | | | -13.919 -11.905 | -5.550 | 1.00 10.13 | À |
| MCTA | 1260 | CG HIS | 249 | | | | Ä |
| ATCM | 1261 | ND1 HIS | 249 | -14.137 -11.129 | -4.486 | 1.00 13.47 | Ţ. |
| MOTA | 1262 | HD1 HIS | 249 | -13.720 -11.294 | -3.611 | 1.00 15.00 | Ä |
| ATOM | 1263 | CD2 HIS | 249 | -14.662 -11.414 | -6.610 | 1.00 10.62 | Ä |
| ATOM | 1264 | NE2 HIS | 249 | -15.317 -10.347 | -6.134 | 1.00 15.51 | À |
| | 1265 | CE1 HIS | 249 | -15.018 -10.142 | -4.821 | 1.00 12.36 | · A |
| ATOM | | | 249 | -10.701 -13.683 | -4.858 | 1.00 23.58 | A |
| ATOM | 1266 | C HIS | | -11.103 -14.729 | -4.359 | 1.00 21.98 | A |
| ATOM | 1267 | O HIS | 249 | | -4.878 | 1.00 29.10 | Ä |
| ATOM | 1268 | N GLY | 250 | -9.398 -13.258 | | | |
| MOTA | 1269 | H GLY | 250 | -9.252 -12.351 | -5.253 | 1.00 15.00 | À |
| ATOM | 1270 | CA GLY | 250 | -8.410 -14.041 | -4.115 | 1.00 24.27 | À |
| ATOM | 1271 | C GLY | 250 | -8.336 -15.372 | -4.743 | 1.00 25.93 | Ä |
| ATOM | 1272 | O GLY | 250 | -8.940 -15.520 | -5.795 | 1.00 29.26 | A |
| ATOM | 1273 | N THR | 251 | -7.594 -16.302 | -4.127 | 1.00 22.38 | A |
| ATOM | 1274 | H THR | 251 | -7.485 -17.038 | -4.804 | 1.00 15.00 | A |
| | 1275 | CA THR | 251 | -7.111 -16.139 | -2.725 | 1.00 21.12 | A |
| ATOM | | CB THR | 251 | -6.988 -17.525 | -1.933 | 1.00 24.76 | A |
| ATOM | 1276 | | 251 | -5.877 -17.641 | -0.981 | 1.00 22.90 | A |
| ATOM | 1277 | OG1 THR | | -6.063 -18.366 | -0.381 | 1.00 15.00 | A |
| MOTA | 1278 | HG1 THR | 251 | | -2.890 | 1.00 22.77 | A |
| ATOM | 1279 | CG2 THR | 251 | -6.968 -18.722 | | 1.00 17.96 | Ä |
| MOTA | 1280 | C THR | 251 | -5.952 -15.158 | -2.473 | | |
| ATOM | 1281 | O THR | 251 | -4.969 -15.043 | -3.213 | 1.00 12.30 | A |
| MOTA | 1282 | N GLY | 252 | -6.241 -14.367 | -1.419 | 1.00 16.85 | A |
| MOTA | 1283 | H GLY | 252 | -7.093 -14.432 | -0.862 | 1.00 15.00 | A |
| ATOM | 1284 | CA GLY | 252 | -5.277 -13.375 | -0.928 | 1.00 13.16 | A |
| ATOM | 1285 | C GLY | 252 | -5.357 -12.058 | -1.670 | 1.00 15.51 | A |
| ATOM | 1286 | O GLY | 252 | -4.580 -11.168 | -1.439 | 1.00 15.18 | A |
| MOTA | 1287 | N PHE | 253 | -6.189 -12.063 | -2.744 | 1.00 16.66 | A |
| ATOM | 1288 | H PHE | 253 | -6.868 -12.805 | -2.761 | 1.00 15.00 | A |
| MCTA | 1289 | CA PHE | 253 | -6.110 -10.892 | -3.651 | 1.00 15.77 | Α |
| ATOM | 1290 | CB PHE | 253 | -6.649 -11.216 | -5.100 | 1.00 17.11 | A |
| | 1291 | CG PHE | 253 | -5.595 -11.840 | -5.994 | 1.00 11.82 | Α |
| ATOM | | CD1 PHE | 253 | -4.385 -11.175 | -6.231 | 1.00 13.69 | Α |
| ATOM | 1292 | CD2 PHE | 253 | -5.845 -13.089 | -6.558 | 1.00 18.59 | A |
| ATOM | 1293 | | 253 | -3.364 -11.771 | -6.993 | 1.00 14.39 | A |
| ATOM | 1294 | | 253 | -4.840 -13.680 | -7.363 | 1.00 21.37 | Α |
| MCTA | 1295 | CE2 PHE | | -3.612 -13.014 | -7.562 | 1.00 15.72 | A |
| MOTA | 1296 | CZ PHE | 253 | -6.740 -9.599 | -3.147 | 1.00 13.88 | A |
| ATOM | 1297 | C PHE | 253 | -6.347 -8.477 | -3.453 | 1.00 14.27 | A |
| ATOM | 1298 | O PHE | 253 | | -2.502 | 1.00 14.00 | A |
| MCTA | 1299 | N THR | 254 | -7.865 -9.837 | | 1.00 15.00 | A |
| MCTA | 1300 | H THR | 254 | -8.079 -10.748 | -2.124 | 1.00 14.09 | Ä |
| MCTA- | 1301 | CA THR | 254 | -8.741 -8.681 | -2.185 | | Ä |
| MCTA | 1302 | CB THR | 254 | -9.908 -8.469 | -3.201 | 1.00 11.66 | Â |
| ATOM | 1303 | OG1 THR | 254 | -9.414 -8.325 | -4.536 | 1.00 13.08 | Â |
| ATCM | 1304 | HG1 THR | 254 | -9.826 -9.054 | -4.992 | | |
| ATOM | 1315 | CG2 THR | 254 | -10.882 -7.321 | -2.885 | 1.00 13.78 | Ÿ |
| ATOM | 1306 | C THR | 254 | -9.270 -8.779 | -0.738 | 1.00 12.36 | A |
| ATOM | 1307 | O THR | 254 | -9. 3 06 -9.695 | -0.240 | 1 00 14.54 | Α |
| ATOM | 1308 | N SER | 255 | -9.007 -7.683 | -0.027 | 1.00 13.42 | A |
| ATOM | 1309 | H SER | 255 | -8.425 -7.021 | -0.490 | 1.00 15.00 | A |
| ATOM | 1310 | CA SER | 255 | -9.032 -7.725 | 1.431 | 1.00 7.59 | A |
| ATOM | 1311 | CB SER | 255 | -7.793 -8.466 | 1.976 | 1.00 6.39 | A |
| ATOM | 1312 | OG SER | | -6.704 -7.560 | 2.041 | 1.00 9.69 | Ä |
| | 1313 | HS SER | 255 | -5.920 -8.031 | 1.741 | 1.00 15.00 | A |
| ATOM | | | 255 | -9.248 -6.341 | 2.085 | 1.00 10.05 | A |
| ATOM | 1314 | | | -9.191 -5.254 | 1.492 | 1.00 15.21 | A |
| ATOM | 1315 | 0 SER | | -9.653 -6.385 | | 1.00 8.54 | A |
| ATOM | 1315 | N PHE | | -9.700 -7.323 | | 1.00 15.00 | A |
| ATCM | 1317 | H PHE | | -10.114 -5.168 | | 1.00 7.94 | A |
| ATOM | 1316 | CA PHE | | -11.605 -5.009 | | 1.00 11.65 | A |
| ATOM | 1319 | CB PHE | 25€ | - 11.003 - 5.009 | | | |
| | | | | | | | |

FIGURE 17W

| MCTA | 1320 | CG | PHE | 256 | -12.376 | -3.524 | 4.235 | | _ |
|-------|------|------|------|-------|-------------|--------|--------|-------------------------|-----|
| ATOM | 1321 | 22: | | 256 | -11.765 | -2.570 | | 1.00 B.71 1.00 11.20 | Ã |
| | | CD2 | | 256 | -13.756 | | 4.533 | | À |
| ATOM | 1322 | 222 | | | | -3.976 | 4.327 | 1.00 6.12 | À |
| ATOM | 1323 | CE1 | PHE | 256 | -12.503 | -1.490 | 5.034 | 1.00 11.49 | À |
| MOTA | 1324 | CE2 | PHE | 256 | -14.514 | -2.849 | 4.734 | 1.00 6.86 | A |
| ATOM | 1325 | CZ | PHE | 256 | -13.862 | -1.657 | 5.211 | 1.00 9.27 | · A |
| MOTA | 1326 | C | PHE | 256 | -9.933 | -5.268 | 5.560 | 1.00 11.92 | A |
| ATOM | 1327 | 0 | PHE | 256 | -10.195 | -6.290 | 6.177 | 1.00 9.43 | Α |
| ATOM | 1328 | N | GLY | 257 | -9.420 | -4.207 | 6.169 | 1.00 10.57 | A |
| ATOM | 1329 | H | GLY | 257 | -9.217 | -3.365 | 5.653 | 1.00 15.00 | A |
| ATOM | 1330 | CA | GLY | 257 | -9.368 | -4.406 | 7.612 | 1.00 11.26 | Ä |
| ATOM | 1331 | C | GLY | 257 | -8.965 | -3.122 | 8.287 | 1.00 11.14 | A |
| ATOM | 1332 | 0 | GLY | 257 | -8.916 | -2.068 | 7.679 | 1.00 10.81 | Ä |
| ATOM | 1333 | N | LEU | 258 | -8.688 | -3.277 | 9.565 | 1.00 12.61 | Â |
| ATOM | 1334 | Н | LEU | 258 | -8.776 | -4.204 | 9.943 | 1.00 15.00 | Â |
| ATOM | 1335 | CA | LEU | 258 | -8.434 | -2.098 | 10.426 | 1.00 14.72 | |
| ATOM | 1336 | CB | LEU | 258 | -9.751 | -1.212 | 10.704 | 1.00 14.72 | A |
| ATOM | 1337 | CG | LEU | 258 | | | | | A |
| | | | | | -10.991 | -1.863 | 11.379 | 1.00 18.02 | A |
| ATOM | 1338 | | LEU | 258 | -12.317 | -1.125 | 11.094 | 1.00 15.05 | A |
| ATOM | 1339 | | LEU | 258 | -10.743 | -2.047 | 12.905 | 1.00 15.42 | A |
| ATOM | 1340 | C | LEU | 258 | -7.737 | -2.525 | 11.709 | 1.00 11.84 | A |
| ATOM | 1341 | 0 | LEU | 258 | -7.851 | -3.690 | 12.096 | 1.00 7.91 | A |
| ATOM | 1342 | N | LEU | 259 | -7.058 | -1.537 | 12.343 | 1.00 11.64 | A |
| ATOM | 1343 | Н | LEU | 259 | -6.883 | -0.685 | 11.844 | 1.00 15.00 | Α |
| ATOM | 1344 | CA | LEU | 259 | -6.581 | -1.780 | 13.714 | 1.00 9.53 | Α |
| ATOM | 1345 | CB | LEU | 259 | -5.155 | -2.417 | 13.831 | 1.00 7.40 | Α |
| ATOM | 1346 | CG | LEU | 259 | -4.194 | -1.621 | 12.931 | 1.00 11.40 | A |
| ATOM | 1347 | CD1 | LEU | 259 | -3.355 | -2.412 | 11.926 | 1.00 7.83 | A |
| ATOM | 1348 | CD2 | LEU | 259 | -3.379 | -0.670 | 13.808 | 1.00 13.30 | A |
| ATOM | 1349 | C | LEU | 259 | -6.652 | -0.497 | 14.531 | 1.00 10.40 | Ä |
| ATOM | 1350 | Ö | LEU | 259 | -6.202 | 0.556 | 14.082 | 1.00 9.73 | Ä |
| ATOM | 1351 | N | LYS | 260 | -7.193 | -0.629 | 15.762 | 1.00 12.00 | Â |
| ATOM | 1352 | Н | LYS | 260 | -7.395 | -1.553 | 16.115 | 1.00 15.00 | |
| ATOM | 1353 | CA | LYS | 260 | -7.069 | 0.521 | 16.693 | | A |
| ATOM | 1354 | CB | LYS | 260 | -8.014 | | | 1.00 13.51 | A |
| | | | | | | 0.312 | 17.885 | 1.00 13.49 | A |
| ATOM | 1355 | CG | LYS | 260 | -8.378 | 1.656 | 18.521 | 1.00 17.16 | Ą |
| MOTA | 1356 | CD | LYS | 260 | -9.435 | 1.456 | 19.596 | 1.00 12.01 | A |
| ATOM | 1357 | CE | LYS | 260 | -10.151 | 2.681 | 20.121 | 1.00 11.41 | A |
| MOTA | 1358 | NZ | LYS | 260 | -9.175 | 3.595 | 20.697 | 1.00 13.33 | A |
| MCTA | 1359 | HZ1 | | 260 | -8.534 | 3.932 | 19.954 | 1.00 15.00 | A |
| ATOM | 1360 | | LYS | 260 | - 9 . 6 9 3 | 4.404 | 21.095 | 1.00 15.00 | A |
| MOTA | 1361 | | LYS | 26C | -3 638 | 3.136 | 21.458 | 1.00 15.00 | Α |
| ATOM | 1362 | C | LYS | 260 | -5.648 | 0.921 | 17.125 | 1.00 16.54 | A |
| MOTA | 1363 | 0 | LYS | 260 | -4.829 | 0.112 | 17.481 | 1.00 15.61 | Α |
| ATOM | 1364 | N | LEU | 261 | -5.353 | 2.199 | 17.015 | 1.00 14.78 | A |
| ATOM | 1365 | H | LEU | 261 | -6.089 | 2.538 | 16.856 | 1.00 15.00 | A |
| MCTA | 1356 | CB | LEU | 261 | -3.705 | 4.005 | 17.185 | 1.00 19.53 | Α |
| MCTA | 1367 | CG | LEU | 261 | -3.177 | 4.309 | 15.787 | 1.00 16.82 | A |
| ATCM | 1368 | CD1 | | 261 | -3.010 | Š.779 | 15.767 | 1.00 12.45 | Α |
| MOTA | 1369 | CD2 | LEU | 261 | -4.010 | 3.906 | 14.577 | 1.00 18.20 | A |
| ATOM | 1370 | c | LEU | 261 | -4.243 | 2.667 | 19.225 | 1.00 20.80 | Ä |
| MCTA | | octi | LEU. | 261 | -5.363 | 2.741 | 19.746 | 1.00 22.59 | Ä |
| ATOM. | 1372 | 0011 | LEU | 261 | -3.221 | 2.696 | 19.913 | 1.00 22.39 | Ä |
| ATOM | 1373 | CA | LEU | 261 | -4.122 | 2.604 | 17.684 | 1.00 28.97 | |
| ATOM | 1374 | - | HOH | 501 | -20.040 | 9.837 | 7.596 | | A |
| ATOM | 1375 | H1 | HCH | 501 | | | | 1.00 16.33 | W |
| ATOM | | | | 3 · · | -19.411 | 10.547 | 7.803 | 1.00 10.00 | W |
| | 1376 | H2 | HCH | 501 | -19.615 | 9.317 | 5.900 | 1.00 10.00 | W |
| ATOM | 1377 | : | HCH | 502 | - 9 . 727 | 11.545 | 10.743 | 1.00 10.94 | W |
| ATOM | 1378 | H1 | нсн | 502 | -10.039 | 11.934 | 9.919 | 1.00 15.00 | W |
| ATOM | 1379 | H1 | нсн | 500 | -10.233 | 12.125 | 11.315 | 1.00 15.00 | W |
| | | | | | | | | | |

FIGURE 17X

| | | _ | 11011 | 503 | -9.158 | 13.188 | 13.681 | 1.00 30. | 64 W |
|--------|--------|----|-------|-----|-------------------|---------|---------|----------|-------|
| MCTA | 1380 | 0 | нон | | -8.715 | 12.529 | 13.277 | 1.00 15. | |
| ATOM | 1381 | Hl | нон | 503 | -8.700 | 13.944 | 13.574 | 1.00 15. | |
| ATOM | 1382 | H2 | нон | 503 | -16.772 | 8.440 | 12.789 | 1.00 12. | |
| MOTA | 1383 | 0 | нон | 504 | | | | | |
| MCTA | 1384 | Hl | HOH | 504 | -17.194 | 9.259 | 12.886 | 1.00 10. | |
| ATOM | . 1385 | H2 | нон | 504 | -15.921 | 8.763 | 12.582 | 1.00 10. | |
| ATOM | 1386 | 0 | нон | 505 | -25.173 | 7.297 | 7.925 | 1.00 47. | |
| MOTA | 1387 | Hl | нон | 505 | -24.690 | 8.064 | 8.239 | 1.00 10. | |
| ATOM | 1388 | H2 | нон | 505 | -25.990 | 7.684 | 7.583 | 1.00 10. | |
| ATOM | 1389 | 0 | нон | 506 | -23.612 | 14.948 | 13.859 | 1.00 36. | |
| ATOM | 1390 | Hl | нон | 506 | -24.160 | 15.702 | 13.605 | 1.00 10. | |
| ATOM | 1391 | H2 | нон | 506 | -23.282 | 15.191 | 14.748 | 1.00 10. | |
| ATOM | 1392 | 0 | нон | 507 | -17.329 | -8.460 | -7.186 | 1.00 34. | |
| ATOM | 1393 | ō | нон | 508 | -18.687 | -7.253 | -3.843 | 1.00 63. | 14 W |
| | 1394 | Ô | нон | 509 | -7.157 | 11.327 | 3.239 | 1.00 22. | 26 W |
| MOTA | 1395 | Õ | нон | 510 | -19.322 | 7.486 | -2.227 | 1.00 37. | 69 W |
| MOTA | | | нон | 511 | -14.645 | -7.711 | -1.931 | 1.00 26. | |
| MOTA | 1396 | 0 | | 512 | -18.377 | -9.754 | 12.556 | 1.00 24. | |
| MOTA | 1397 | 0 | нон | | 0.030 | | -13.455 | 1.00 26. | |
| MOTA | 1398 | 0 | нон | 513 | -8.938 | 5.945 | 22.862 | 1.00 34. | |
| ATOM | 1399 | 0 | нон | 514 | | -4.922 | -7.247 | 1.00 41. | |
| MOTA | 1400 | 0 | нон | 515 | -29.446 | 10.220 | 10.038 | 1.00 47. | |
| MOTA | 1401 | 0 | нон | 516 | -12.982 | -9.377 | 7.242 | 1.00 60. | |
| MOTA | 1402 | 0 | нон | 517 | -21.797 | | | 1.00 40. | |
| ATOM | 1403 | 0 | HOH | 518 | -7.867 | 8.165 | 19.484 | | |
| ATOM | 1404 | 0 | HOH | 520 | -15.588 | | 14.628 | 1.00 63. | |
| ATOM | 1405 | 0 | HOH | 521 | -21.844 | 7.778 | 20.415 | 1.00 35. | |
| ATOM | 1406 | 0 | нон | 522 | -6.555 | | -15.790 | 1.00 33. | |
| ATOM | 1407 | 0 | нон | 523 | -9.046 | -13.476 | -8.051 | 1.00 44. | |
| ATOM | 1408 | 0 | нон | 524 | -17.413 | -9.311 | 17.071 | 1.00 34. | |
| ATOM | 1409 | 0 | нон | 525 | -23.838 | 4.781 | 19.884 | 1.00 37. | |
| ATOM | 1410 | Ō | нон | 526 | -26.323 | 15.525 | 10.379 | 1.00 72. | |
| ATOM | 1411 | ō | нон | 527 | -3.167 | -13.749 | -10.820 | 1.00 43. | |
| ATOM | 1412 | Ö | нон | 528 | -0.470 | 2.513 | 17.943 | 1.00 63. | 68 W |
| ATOM | 1413 | Ö | нон | 529 | -5.580 | -12.778 | -14.864 | 1.00 47. | |
| MOTA | 1414 | Ö | нон | 530 | -2.641 | 7.004 | 2.495 | 1.00 18. | 07 W |
| ATOM | 1415 | ŏ | нон | 531 | -6.472 | 12.847 | 0.156 | 1.00 24. | 96 W |
| | 1416 | Ö | нон | 532 | -10.363 | -16.426 | -0.360 | 1.00 63. | 56 W |
| ATOM | | Ö | нон | 533 | | -17.183 | | 1.00 67. | 67 W |
| ATOM | 1417 | 0 | нон | 534 | -4.774 | 9.073 | -0.651 | 1.00 23. | |
| ATOM | 1418 | | нон | 535 | | -13.857 | 6.913 | 1.00 32. | |
| MOTA | 1419 | 0 | нон | 536 | -23.062 | 3.270 | 0.454 | 1.00 52. | |
| ATOM | 1420 | 0 | нон | 537 | -25.906 | 9.022 | 16.986 | 1.00 44. | |
| ATOM | 1421 | 0 | | 538 | -21.729 | 16.972 | 17.027 | 1.00 53. | |
| ATOM | 1422 | 0 | нон | | -9.084 | 11.806 | 17.034 | 1.00 70. | |
| ATOM | 1423 | 0 | нон | 539 | | -13.296 | 15.207 | 1.00 35. | |
| MOTA | 1424 | 0 | нон | 540 | | 13.255 | 17.989 | 1.00 67. | |
| ATOM | 1425 | 0 | нон | 541 | -6.068 -20.593 | -11.039 | -9.003 | 1.00 96. | |
| MOTA | 1426 | 0 | нон | 542 | | 13.397 | 1.269 | 1.00 35. | |
| ATOM | 1427 | 0 | нон | 543 | -15.926 | | -2.353 | 1.00 43. | _ |
| ATOM | 1428 | 0 | нон | 544 | -24.591 | -7.285 | | 1.00 53. | |
| MCTA | 1429 | ၁ | HOH | 545 | -25.859 | | -15.747 | 1.00 56 | |
| MOTA | 1430 | 0 | HOH | 546 | -23.074 | -1.533 | 11.026 | | · • - |
| ATOM . | 1431 | 0 | нон | 548 | -8.941 | | -12.394 | 1.00 64 | |
| MCTA | 1432 | С | HCH | 549 | -14.150 | | -12.250 | 1.00 41. | . – – |
| MCTA | 1433 | 0 | нон | 550 | -14.274 | -0.613 | 18.441 | 1.00 56 | |
| ATOM | 1434 |) | нон | 551 | -12.241 | | 8.637 | 1.00 80 | |
| ATOM | 1435 | C | нон | 552 | -10.316 | | 10.166 | 1.00 39 | . • - |
| ATOM | 1436 | 0 | HOH | 553 | -15.367 | 10.941 | 14.659 | 1.00 40 | |
| ATOM | 1437 | 0 | нон | 554 | -2.322 | | | 1.00 33 | |
| ATOM | 1438 | 0 | нон | 555 | | -14.875 | | 1.00 52 | |
| MOTA | 1439 | Ö | нон | 556 | -22.120 | | | 1.00 38 | .55 % |
| | | | | | | | | | |

FIGURE 17Y